Fuel Effects on Exhaust Emissions from Onroad Vehicles in MOVES3

EPA United States Environmental Protection Agency

Fuel Effects on Exhaust Emissions from Onroad Vehicles in MOVES3

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.

EPA United States Environmental Protection Agency

EPA-420-R-20-016
November 2020

Contents

1 Introduction 4
2 "Base" and "Target" Gasolines 6
2.1 Base Gasoline 7
2.2 Target Gasolines 7
2.2.1 Relevant Database Tables 8
3 Fuel Sulfur Effects 9
3.1 Introduction 9
3.2 The MOBILE6 Sulfur Model (M6Sulf) 10
3.2.1 Data Used in Developing the M6Sulf Model 10
3.2.2 Analysis of Short-Term Sulfur Effects 12
3.2.3 Analysis of Long-Term Sulfur Effects 19
3.2.4 Application in MOVES 22
3.3 Tier 2 Low Sulfur Model (T2LowSulf) 29
3.3.1 Background 29
3.3.2 Data Used in Developing the T2LowSulf Model 29
3.3.3 Data Analysis and Results 32
3.3.4 Application in MOVES 48
3.4 Results: Sulfur Effects in MOVES3 50
4 Use of the Complex Model (for CO Emissions) 53
4.1 Overview of the Complex Model 53
4.2 Application of the Complex Model 56
5 Use of the EPA Predictive Model (HC and NO_x Emissions) 58
5.1 Data Used in Developing the EPA Predictive Model 58
5.2 Analytic Approaches 58
5.2.1 Standardization of Fuel Properties 59
5.3 Application in MOVES 62
6 Gasoline Fuel Effects for Vehicles certified to Tier 2 Standards (EPAct Models: HC, CO, NO_x, PM) 63
6.1 Introduction: the EPAct Project 63
6.2 Analysis and Model Fitting 68
6.2.1 Standardizing Fuel Properties 68
6.2.2 Fitting Procedures 70

6.3 Scope and Implementation 76
6.4 De-standardization of Model Coefficients 77
6.4.1 De-standardizing Linear Terms 77
6.4.2 De-standardizing 2nd-order Terms 78
6.5 Fuel Effect Adjustments 81
6.6 The Database Table "GeneralFuelRatioExpression" 83
6.6.1 Examples 83
7 High-Level Ethanol Blends (E85) 86
7.1 Introduction 86
7.2 Data Analysis and Results 87
7.3 Application in MOVES 93
7.3.1 Example MOVES Results 96
8 Biodiesel Blends 99
8.1 Pre-2007 Diesel Engines 99
8.2 2007 and later Diesel Engines 99
8.3 Modeling Biodiesel 99
9 Sulfate and Sulfur Dioxide Emissions 100
9.1 Introduction 100
9.2 Sulfate Calculator Summary 101
9.3 Gasoline Vehicles 104
9.3.1 Pre-2004 Light-duty Gasoline Vehicles 104
9.3.2 2004 and later Light-duty Gasoline Vehicles 105
9.3.3 High Ethanol Blend (E85) Gasoline Vehicles 106
9.3.4 Motorcycles Heavy-duty Gasoline Vehicles 106
9.4 Diesel Vehicles 106
9.4.1 Pre-2007 Diesel Vehicles 106
9.4.2 2007 and Later Technology Diesel Vehicles 107
9.5 Compressed Natural Gas 107
9.6 Example Comparisons 108
9.7 Sulfur Dioxide Emissions Calculator 110
9.8 Summary 112
Appendix A Derivation of the Sulfate Equation and Parameters 114
Appendix B Estimation of Weight % Oxygenates for the Complex and Predictive Models 129

Appendix C High Ethanol (E85) Fuel Adjustments and HC species VOC and NMOG..... 130
10 References..... 133

1 Introduction

The MOVES 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 (LPG), "Ethanol (E-85)" and "electricity." The "Ethanol" category includes blends of ethanol and gasoline in which the ethanol fraction exceeds 70 vol.%. This document discusses adjustments or other calculations designed to account for the effects of changes in fuel properties on exhaust emissions of THC, CO, NO_x and PM. Similar calculations applied to emissions of air toxics and evaporative emissions are discussed in separate reports.[1,2] Clearly, fully electrified vehicles do not emit exhaust pollutants, and will not be further discussed in this report.[a] Note that MOVES3 estimates emissions using LPG only for the NONROAD component of the model.[b]

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. MOVES estimates "gasoline" emissions for gasoline blends with ethanol up to 15 vol.%. The treatment for ethanol (E-85), diesel and CNG is much simpler.

Estimation of emissions from gasoline plays a very important role in MOVES. 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.[2]

Ethanol mandates are reflected in the model, including the renewable fuels standards (RFS1 and RFS2[60]). The MOVES fuel supply currently reflects the fact that most gasolines in the U.S. contain approximately 10 vol.% ethanol. In addition, MOVES includes the capability to model the fuel effects of gasolines containing up to 15 vol.% ethanol, i.e., "E15" fuels; however, these fuels are intended for specific modeling scenarios and are not included in the default fuel supply. Also, although it was used in some historical gasoline blends, MOVES does not model emissions from gasoline with methyl-tertiary-butyl-ether (MTBE), but instead substitutes equivalent ethanol blending to account for oxygenate requirements in years where MTBE was present. The construction and composition of the default fuel supply is described in greater detail in a separate report.[3]

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,

[a] MOVES does not model upstream or lifecycle emissions.

[b] It is visible in the *fuelType* table and in the GUI due to sharing of tables between the onroad and NONROAD components of the model.

maximum and average sulfur levels were reduced from 300 to 80 and 120 to 30 ppm from 2004 and 2006, respectively.[4] Under the Tier 3 program, further reductions to an average gasoline sulfur level of 10 ppm were achieved starting in 2017.[5]

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 (the typical fuel in-use during base rate emission collection), and "target" emissions, intended to reflect the set of "target" fuels in the areas and periods covered in a MOVES run. This "base" reference fuel has been updated in MOVES3 to reflect more recent exhaust emission testing and analysis conducted since the release of the previous model version. The concept and updated definitions of the base gasoline properties are discussed below in Section 2.

During a run, MOVES combines emission rates and vehicle 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 gasoline 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 gasoline 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 less than 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 all gasoline 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 all gasoline vehicles manufactured 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 are described in Chapter 6.

In MOVES, fuel sulfur plays yet another role in estimating emissions of sulfate (SO_4) as a component of the non-elemental-carbon component of $PM_{2.5}$. The 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 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, MOVES estimates emissions of sulfur dioxide (SO_2) as a function of gasoline consumption and sulfur level. Unlike the sulfate calculation, the SO_2 calculation assumes that all emissions are contributed by the fuel. As with the sulfate calculation, the SO_2 calculation uses the same structure for all fuels. Assumptions specific to gasoline are shown in Table 9-3.

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 either gasoline or "high-level" ethanol blends are designated as flexible-fuel or "flex-fuel" vehicles (FFVs). MOVES estimates 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.

Some sections of a draft version of this document underwent external peer review. The draft reports, peer reviewer comments, the Agency's responses, and related peer-review for the updates made to MOVES2014[6] and MOVES3[7] are provided on EPA's Science Inventory webpage.

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 (excluding the Tier 2 Sulfur Model, see Section 3.3.4). The research and analysis underlying 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.

MOVES3 uses a single base fuel for adjustments made based on the Complex, Predictive, and EPAct models. This base fuel was updated in the MOVES3 model to better represent the fuels seen in-use as part of the study deriving base emission rates.[8] The properties of this fuel are defined in the database table *BaseFuel*, and are further described in sub-section 2.1.

2.1 Base Gasoline

For gasoline, MOVES3 uses a single base fuel for the calculation of fuel adjustments for non-sulfur properties. This fuel is assumed to represent the "typical" in-use gasoline seen in the Denver metropolitan area between calendar years 2009 and 2017. The emission rates for gaseous emissions from light-duty vehicles are based on random evaluation samples from the Denver Inspection and Maintenance (I/M) Program during this time period and from Denver remote sensing data (RSD) in a similar time period. The development of these "I/M reference rates" (meanBaseRateIM) is described in detail in a separate report.[8] Because fuel properties for individual vehicles in the I/M lanes and RSD testing are unknown, we assume that the "averaged" fuel properties, based on refinery batch data in the same area during the same time period, are representative and can be associated with the average emission rates. The properties of this fuel are shown in Table 2-1 below and are represented by fuelFormulationID 99 in the MOVES3 *fuelFormulation* database table.[c]

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 gasolines vary by county, year, and month. The MOVES 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 2060. 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.[3]

[c] Although the MOVES3 *baseFuel* database table also contains base fuels with *fuelFormulationID*s 96 and 98 for model years 2001-2050, this year range has been entirely superseded by the fuel adjustment models contained in the *generalFuelRatioExpression* database table and thus the properties of these two fuels do not have any effect on model results (see Section 6.6).

Table 2-1. Properties of the MOVES3 Base Gasoline.

Fuel Property Name	Fuel Property Value
Fuel Sub-Type	E-10 (fuelSubtypeID 12)
fuelFormulationID	99
RVP (psi)	8.8
Sulfur Level (ppm)	30.0
Ethanol Volume (%)	10.0
Aromatic Content (%)	25.77
Olefin Content (%)	8.44
Benzene Content (%)	0.65
E200 (%)	47.61
E300 (%)	84.89
T50 (°F)	212.3
T90 (°F)	321.7
Volume to percent Oxygen (%)	0.3653

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 fuel used by MOVES3 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.[1]

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 6.6.

The additional tables listed below are described in the Fuel Supply report:[3]

FuelFormulation,
FuelSupply,
RegionCounty,
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 "clean" catalysts.

This chapter describes how MOVES 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 MOVES assumes that there is no direct impact of fuel sulfur on criteria emissions from diesel vehicles. Note also that emissions of sulfate (SO_4) and sulfur dioxide (SO_2) are discussed in Chapter 9.

MOVES 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 MOVES.

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 Study[12]–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 Study[13]–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.

T_{50}/T_{90}/Sulfur Study[14]–The study was designed to investigate possible non-linear impacts of the fuel distillation parameter T_{90}, interactive impacts of two fuel distillation parameters (T_{50} and T_{90}) and sulfur on emissions from light-duty vehicles. Three vehicle fleets were tested: 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 T_{90} set and a high T_{90} set with approximate sulfur levels of 33 and 317 ppm.

API Extension Fuel Set[15]–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 Study[16]–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 Study[17]–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" Study[18]- 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 Study[19]– 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 Study[20] –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 21vehicle 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 MOVES 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 3.2.2.2, 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 is 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 T_{50}/T_{90} sulfur data set in the current analysis. Inspection of the T_{50}/T_{90} sulfur data shows somewhat muted HC effects and much lower NO_x effects for sulfur variations. The T_{50}/T_{90} 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 T50/T90 Sulfur Study, 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

[1]Please 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,

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

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),

$f_{T1,330}$ = 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

3.2.2.2 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 to 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	-5.0	1.4	10.0

* CO emissions were not in the original RFG Complex Model. The CO model was developed separately (using the same statistical techniques used to construct the RFG Complex Model) and is discussed in SAE paper 961214[13].

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 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	NO_x	HC	CO	NO_x
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	NO_x	HC	CO	NO_x
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 MOVES, 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 "*sulfurmodelname*" 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 "sulfurmodelname" 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" ($C_{short,target}$) 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, $C_{short,basis}$, is the correction factor for the base sulfur (*sulfurBasis* variable in the *SulfurBase* table) level. The sulfur basis ($x_{S,basis}$) is always set at 30 ppm.

$$C_{short,target} = \exp\left(\beta \ln x_S\right) \quad \textbf{Equation 3-2}$$

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

$$C_{short,target} = \exp\left(\beta\, x_S\right) \quad \textbf{Equation 3-4}$$

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

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

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

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 MOVES (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.

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

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 only to "LEV" and later (2001+ model year) vehicles, and apply only to target fuel sulfur levels greater than 30 ppm sulfur. For model years 2000 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

$$A_{S,Irr} = \exp\left(\phi \ln x_{S,cap}\right) \qquad \textbf{Equation 3-8}$$

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 (A2, 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]

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

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:

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

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

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.

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

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.

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

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.

$$A_{S,combined} = (1 - f_{GPA})A_{S,3} + f_{GPA}A_{3,GPA}$$ **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 MOVES 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.

$$A_{S,3}^{target} = (1 - w_{high})A_{S,3,normal}^{target} + w_{high}A_{S,3,high}^{target}$$
$$A_{S,3}^{base} = (1 - w_{high})A_{S,3,normal}^{base} + w_{high}A_{S,3,high}^{base}$$ **Equation 3-15**

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

$$A_{3,GPA}^{target} = (1 - w_{high})A_{3,GPA,normal}^{target} + w_{high}A_{3,GPA,high}^{target}$$
$$A_{3,GPA}^{base} = (1 - w_{high})A_{3,GPA,normal}^{base} + w_{high}A_{3,GPA,high}^{base}$$ **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 2001-2060.

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

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

Equation 3-17

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 Section 3.2.

Eqn	Eqn(GPA)	Symbol	Name	Type (*DB table*)	Description
3-2, 3-3, 3-4, 3-5	3-10	β	*sulfurCoefficient*	DB input (S*ulfurmodelcoeff*)	Regression coefficient for short-term sulfur effects (log-log or log-linear).
3-2	3-10	x_S	*sulfurTarget*	DB Input (*FuelFormulation*)	"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		$x_{S,basis}$	*sulfurBasis*	DB input (*SulfurBase*)	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		$A_{S,long}$	*sulfurLongCoeff*	DB input (*M6SulfurCoeff*)	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		$x_{S,cap}$	*maxIRFactorSulfur*	DB input (*M6SulfurCoeff*)	Maximum S level for which "irreversibility effect" is calculated. Varies by specified model-year groups.
3-8		ϕ	*sulfurCoefficient*	DB input (S*ulfurmodelcoeff*)	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}	sulfurIRFactor	DB input (*M6SulfurCoeff*)	
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 2001-2060.

3.3 Tier 2 Low Sulfur Model (T2LowSulf)

The M6Sulf model, described above, is used in MOVES 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," is used, based on additional data collected since the M6Sulf model was created.

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 MSAT[25] and Umicore[24] 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 EPAct/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 3-17 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 Level[1]
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 Fuel[1]
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 provides the key information for assessing the in-use effect of target sulfur levels on emissions over time as vehicles accumulated mileage. Only the analyses pertaining to the “sulfur level” data are discussed in the following section since it’s the most

relevant in the context of MOVES. 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 (CH_4), 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

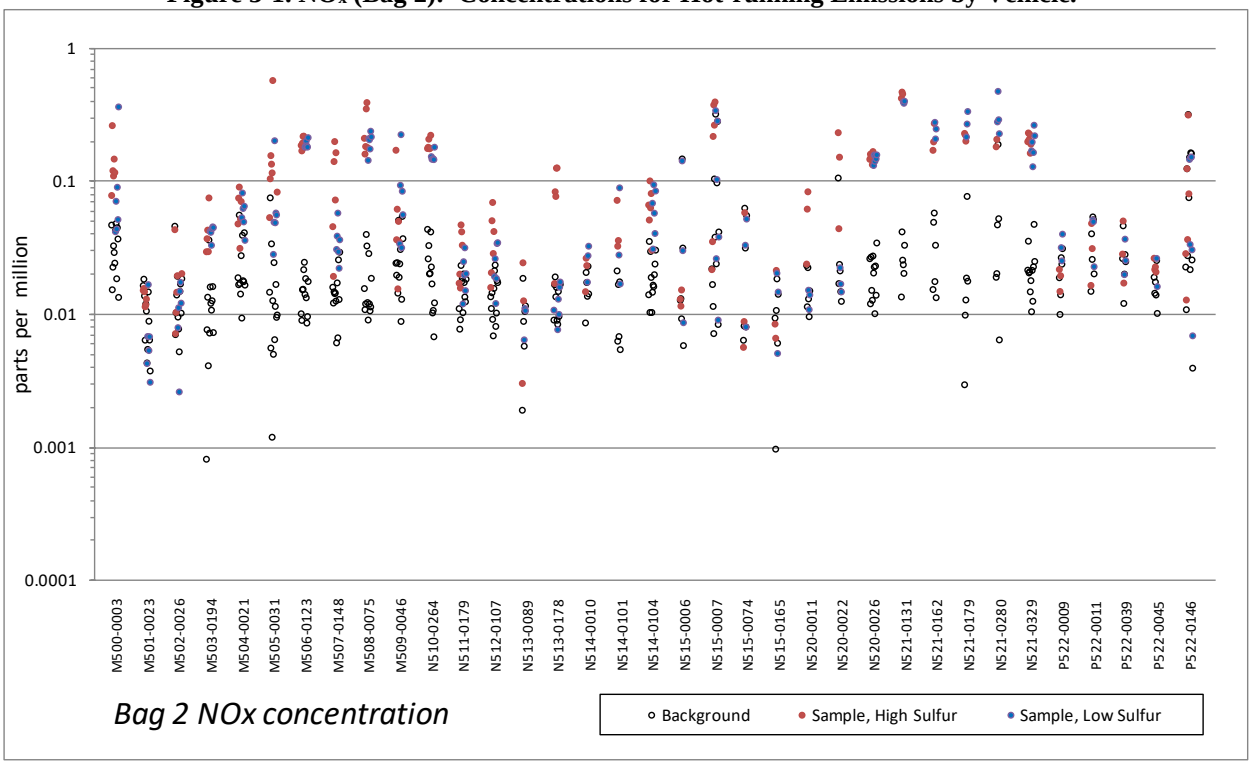
The graphical examination of the "sulfur level" dataset revealed the presence of very low emission measurements from some pollutants and bags including NO_x Bag 2. Since uncertainty associated with these low measurements could potentially affect the outcome of the analysis, it was important to understand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

$$\boldsymbol{Y_i = X_i\beta + Z_i u_i + \varepsilon_i} \qquad \textbf{Equation 3-18}$$

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.

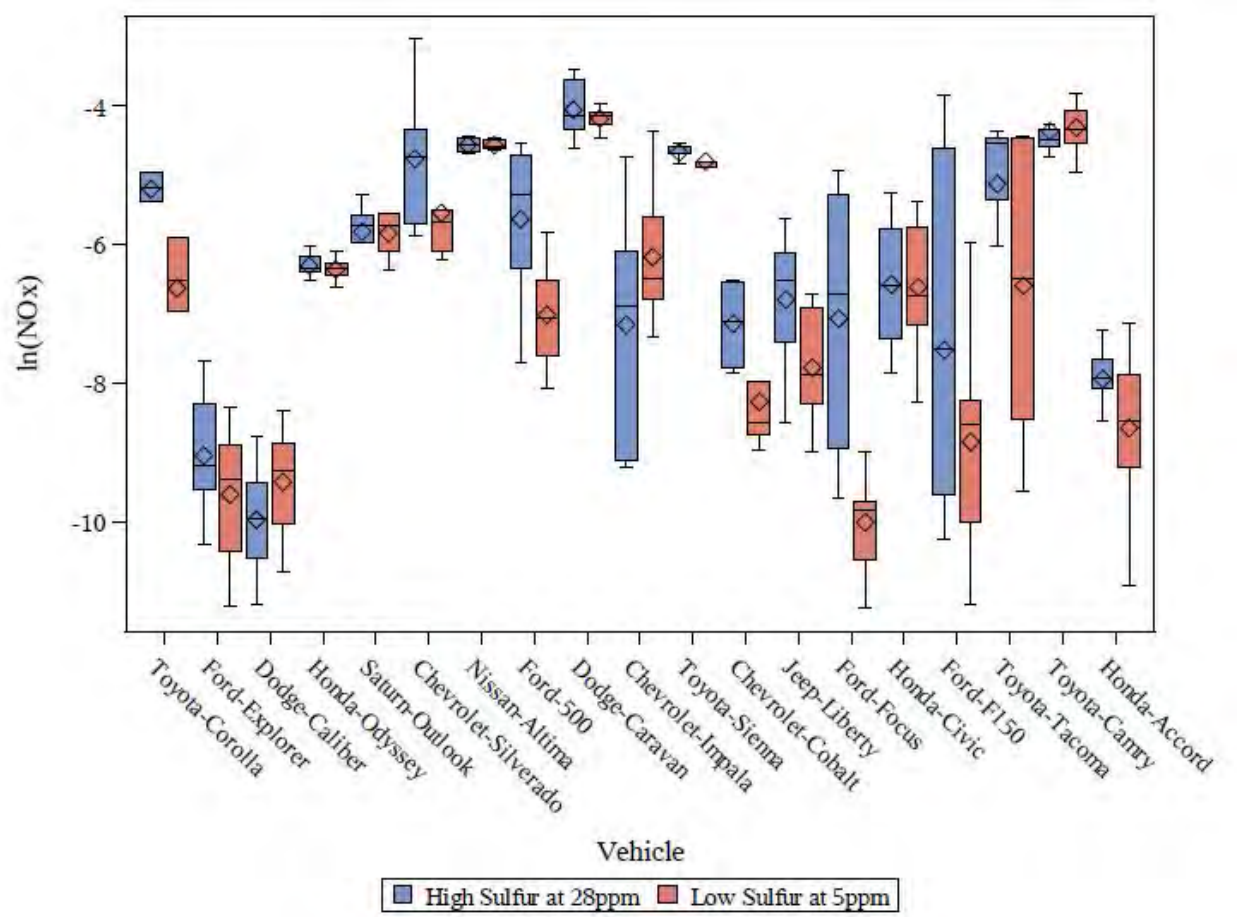
In developing the mixed model, a top-down model fitting strategy was used, similar to previously established methods.[35,36] The first step was to start with a "saturated" or full model, which included all candidate fixed effects to allow unbiased estimation of the random effect estimates. Next, we selected 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).



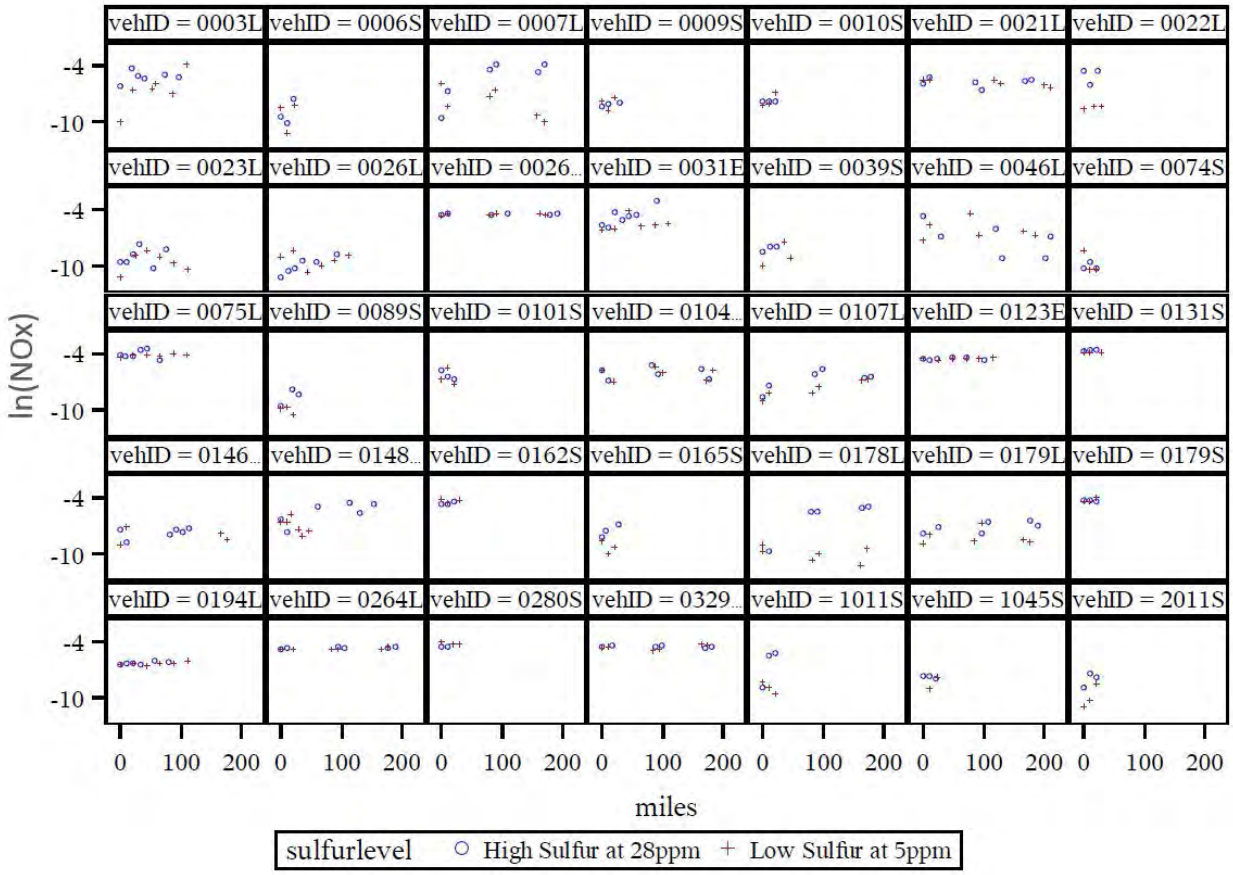
In the dataset, the numbers of tested vehicles are not the same across vehicle families. Considering the differences in numbers of unique vehicles in each vehicle family and the presence of variability among vehicle families illustrated in Figure 3-2, each vehicle family was considered as a random effect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

$$\boldsymbol{R_i = Var(\epsilon_i) = \begin{bmatrix} \sigma^2 & \sigma^2\rho & \sigma^2\rho^2 & \cdots & \sigma^2\rho^{n-1} \\ \sigma^2\rho & \sigma^2 & \sigma^2\rho & \ldots & \sigma^2\rho^{n-2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \sigma^2\rho^{n-1} & \sigma^2\rho^{n-2} & \sigma^2\rho^{n-3} & \ldots & \sigma^2 \end{bmatrix}} \qquad \textbf{Equation 3-19}$$

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	Effect[1]	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.

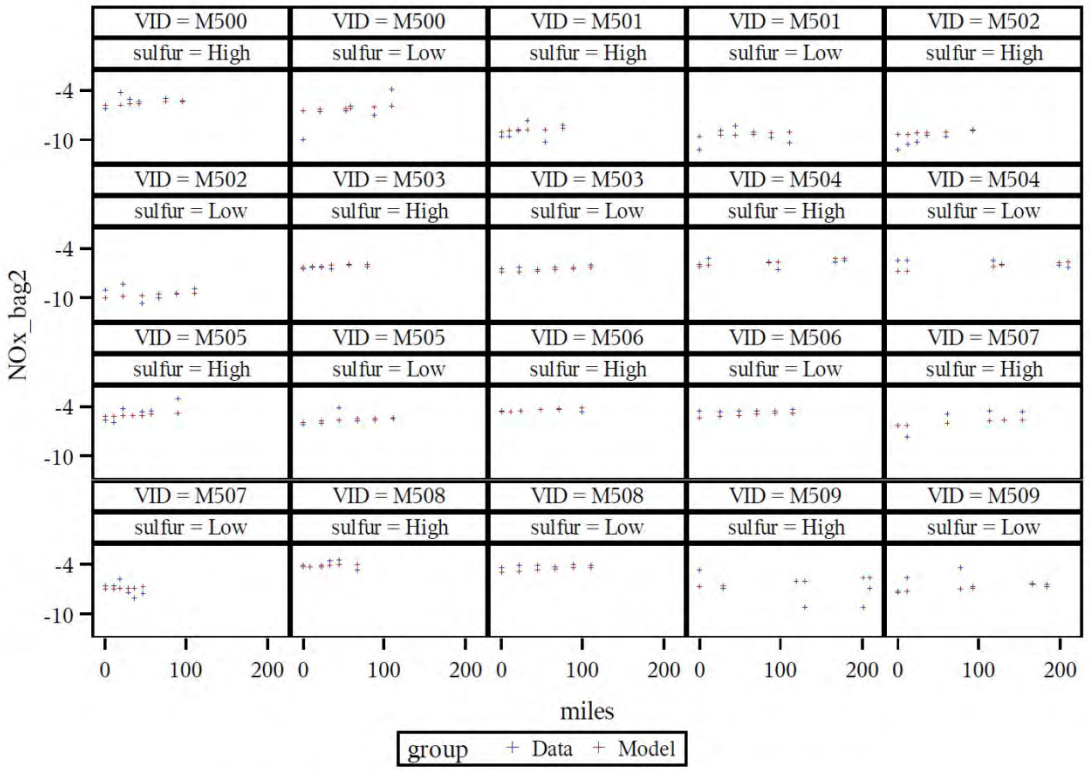
Table 3-22. Likelihood Ratio Test for Bag 2 NO_x Model.

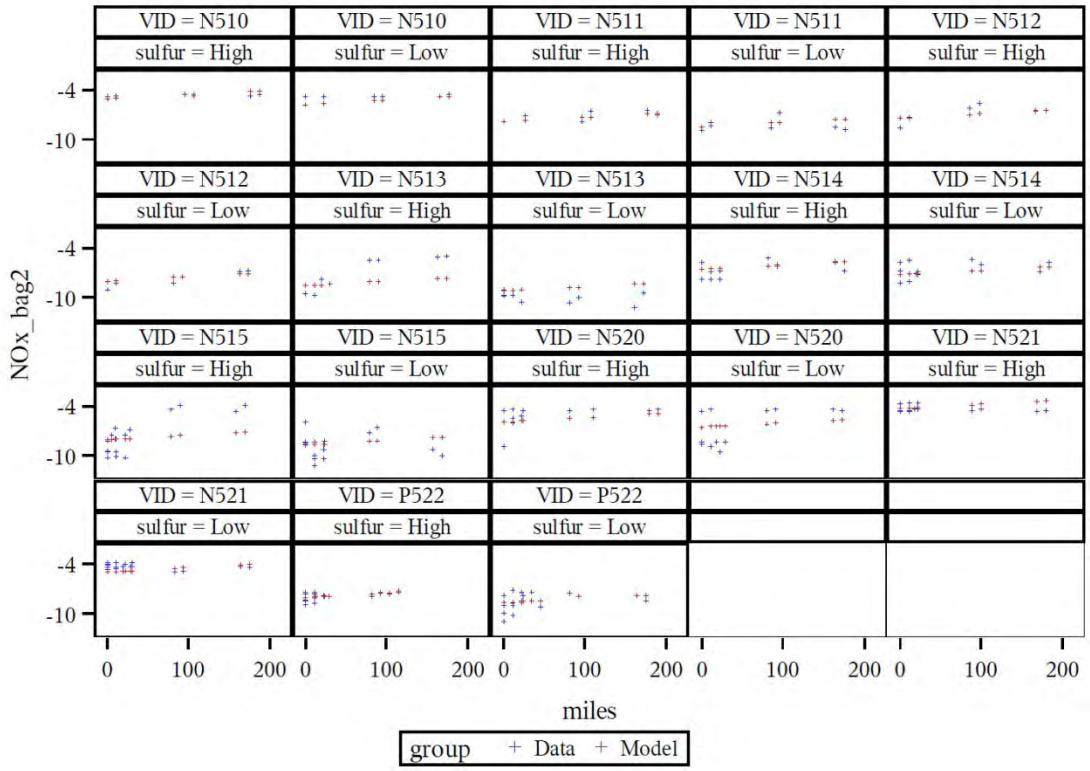
	Fixed effects	-2 Res Log Likelihood	p-value (χ^2)
Model 4	slevel, miles	991.6	0.1213
Model 5	slevel	994	

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 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).

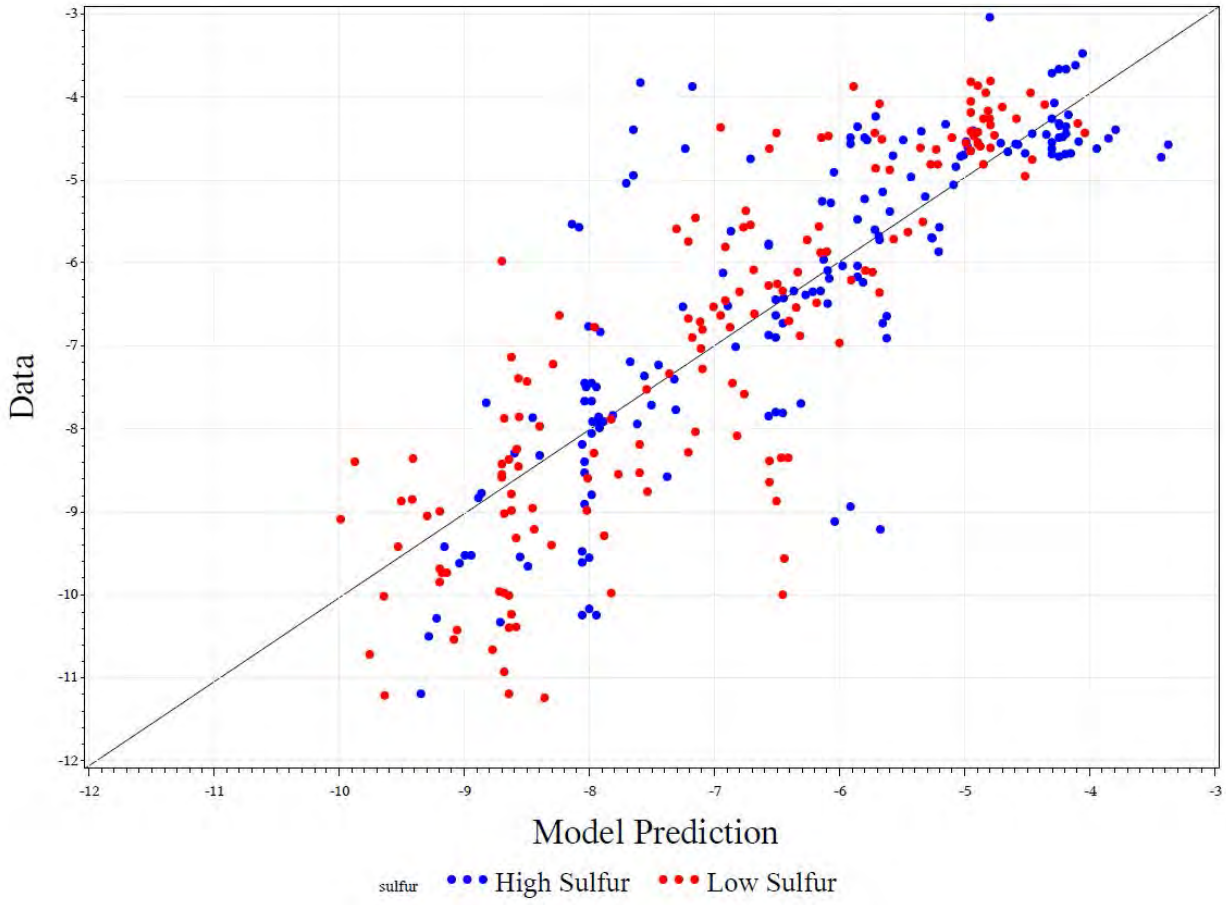


Table 3-23 summarizes the final models selected for all pollutants and bags, applying the same statistical methodology described for Bag 2 NO_x. For all models, the sulfur-level and mileage interaction terms were not significant, and the change in emissions from reducing the fuel-sulfur from 28 ppm to 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 Effects[1]
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 (*p*-value)	**THC (*p*-value)**	**CO (*p*-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 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.

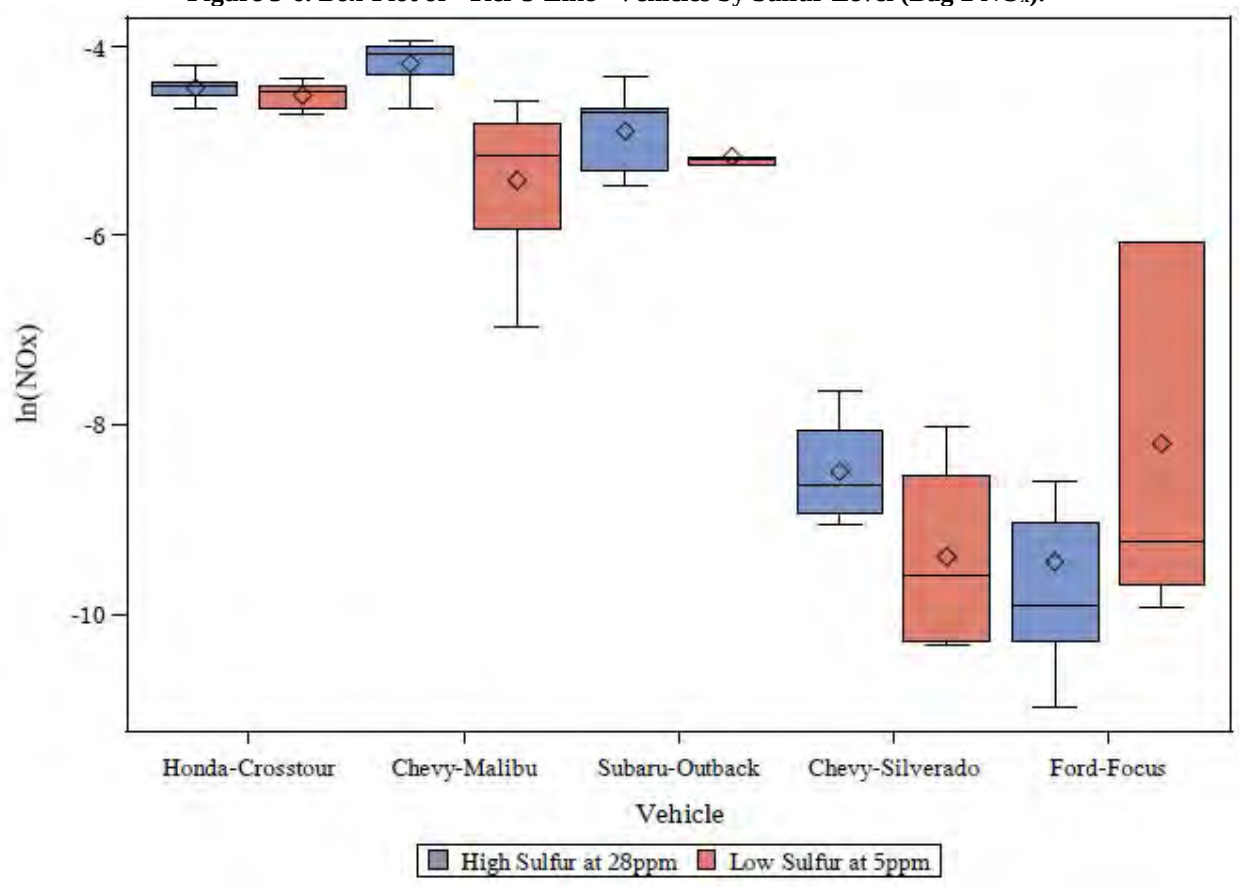
Table 3-25. Description of "Tier 3-like" Vehicles in the "Sulfur Level" Data.

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 3 equivalent" 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 3 equivalent" 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

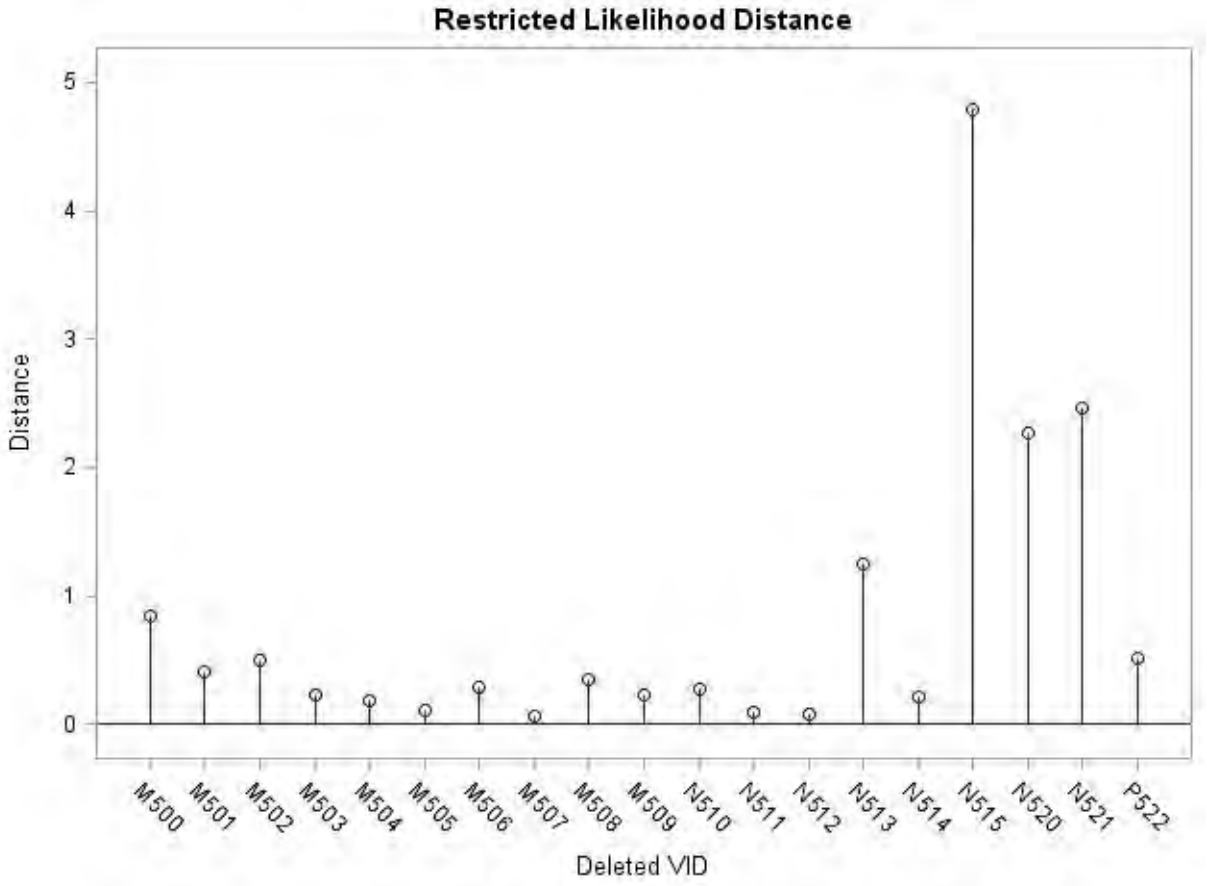
In order to assess the impact of substituting for censored values, models with and without imputed values for Bag 2 NO_x were compared. For the model without imputed values, the mixed model was re-fit using a new dataset with all imputed values removed, consisting only of actual measurements. Based on 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 were incorporated into MOVES3 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.

$$A_S = 1.0 - \beta_S\left(S_{base} - x_S\right)$$ **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, xS 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. Subsequently, for light-duty passenger cars (sourceType 21) in model year group 2017-2060, the sulfur base is set at 10 ppm due to the assumption that Tier 3 Vehicle Standard is enabled by Tier 3 vehicles running on 10 ppm sulfur. This prevents double-counting of the impacts of low levels of sulfur in fuels for Tier 3 vehicles. Similarly, light-duty trucks (sourceType 31 and 32) in model year group 2018-2060 are also set to a sulfur base of 10 ppm, with the additional year accounting for a lag in low sulfur phase-in for these vehicles. Vehicles in heavier weight classes (sourceType 41 and above) continue through 2060 with a sulfur base of 30 ppm. 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 ("*generalFuelRatioExpression*"). This table consolidates the two sulfur models (M6Sulf and T2LowSulf) for MYG 2001-2016 and 2017-2060, and the other fuel-effect models (i.e., EPAct 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 provided in Section 6.6..

3.4 Results: Sulfur Effects in MOVES3

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.

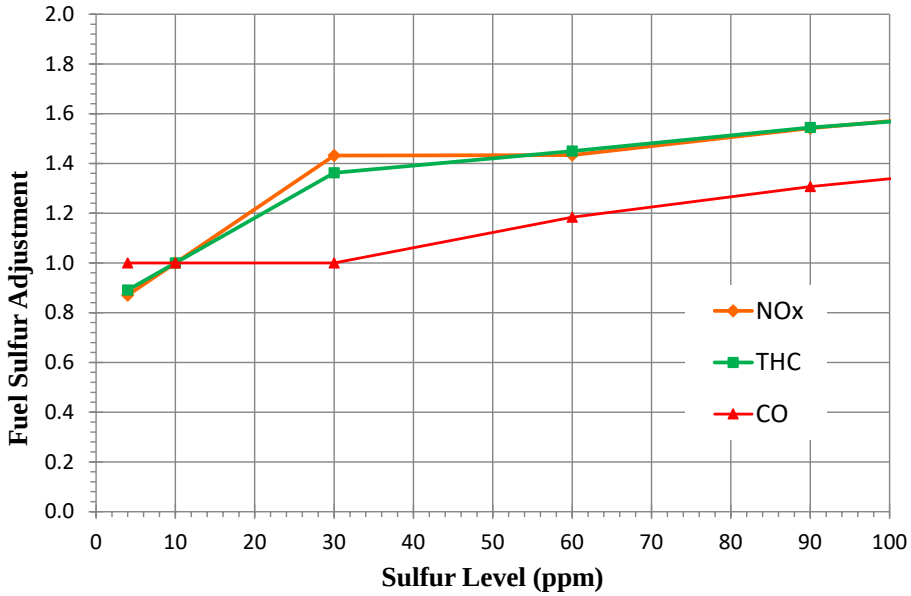


Figure 3-9. Relative Fuel Sulfur Effect for Running Exhaust Emissions for MYs 2001 to 2016, normalized to a sulfur level of 30 ppm.

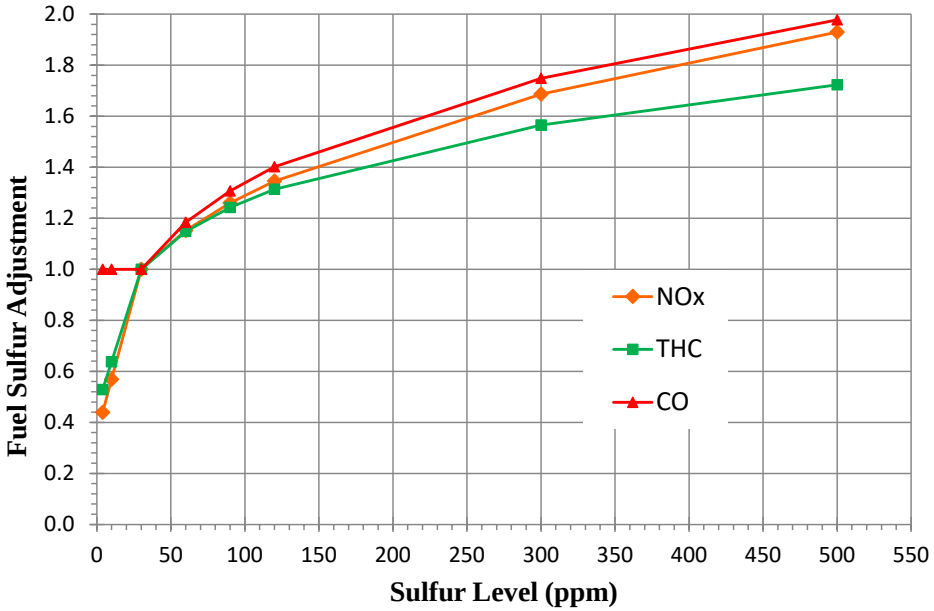


Figure 3-10. Relative Fuel Sulfur Effect for Running Exhaust Emissions for MY 1996, normalized to a sulfur level of 90 ppm.

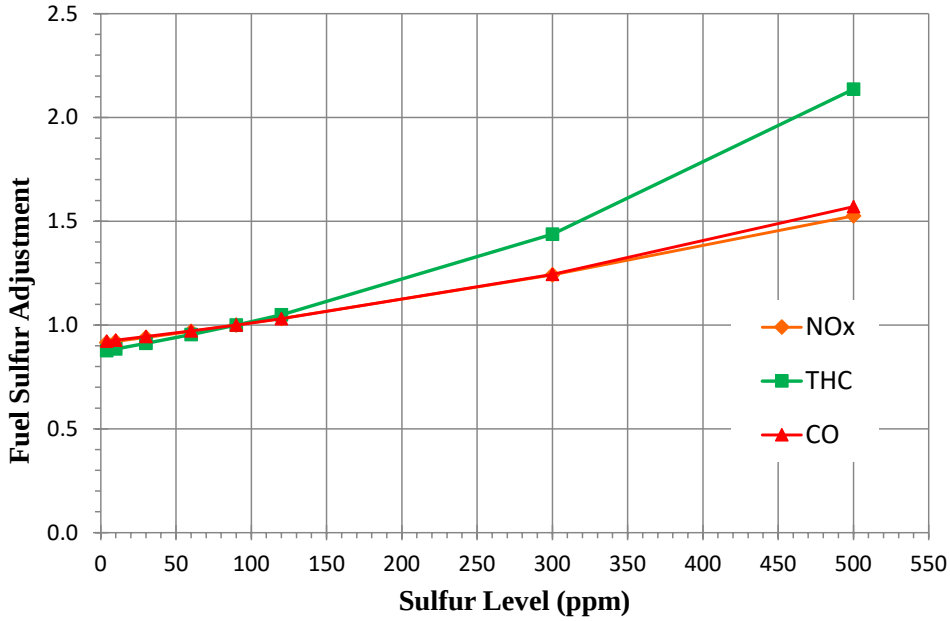
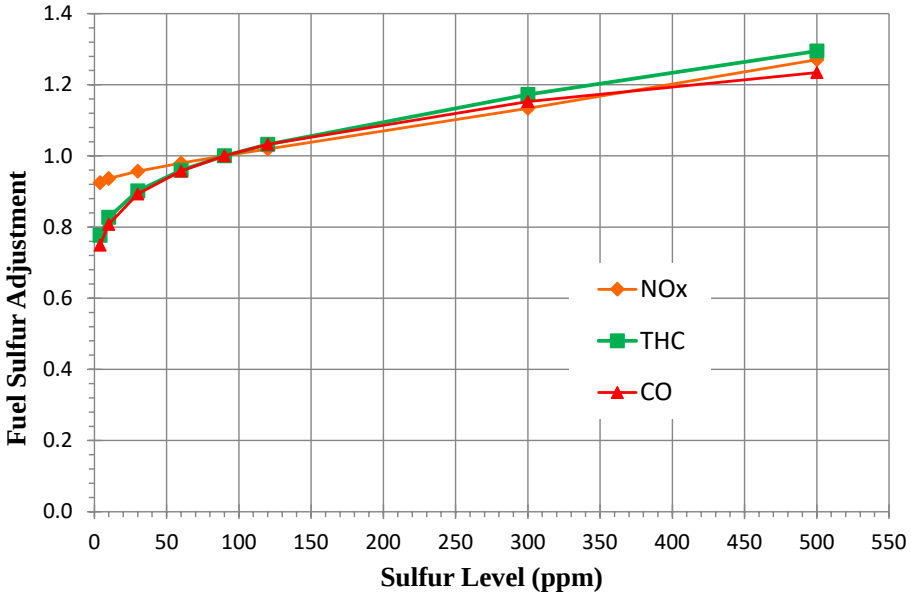


Figure 3-11. Relative Fuel Sulfur Effect for Running Exhaust Emissions for MY 1988, normalized to a sulfur level of 90 ppm.



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[d] 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.

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

The mean values used for centering all individual fuel property values are presented in

[d] For additional details on the mean fuel property values used for centering the terms in the complex model, see *Air Toxic Emissions from On-road Vehicles in MOVES3.*[1]

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	RVPSQR	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 2). 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 $\mathbf{X\beta_{target}}$ and $\mathbf{X\beta_{base}}$ for estimates on the target and base fuels, then the fractional difference in emissions is given by

$$f_{\text{adj}} = \frac{\exp\left(\mathbf{X\beta}_{\text{target}}\right)}{\exp\left(\mathbf{X\beta}_{\text{base}}\right)} - 1.0 \qquad \textbf{Equation 4-2}$$

The expression in Equation 4-2 is evaluated for the same 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.

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

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.

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

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. 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).[e]

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

[e] 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, second-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 × T90 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.

$$Z_{ARO} = \frac{\left(x_{ARO,i} - \bar{x}_{ARO}\right)}{s_{ARO}} \qquad \textbf{Equation 5-1}$$

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).

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

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

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 ln*Y* 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 second-order quadratic and interaction terms, respectively.

$$\ln Y = \beta_0 + \beta_{\mathrm{OXY}} Z_{\mathrm{OXY}} + \beta_{\mathrm{ARO}} Z_{\mathrm{ARO}} + \cdots + \beta_{\mathrm{RVP}} Z_{\mathrm{RVP}} + \cdots$$
$$\cdots + \beta_{\mathrm{T50SQR}} Z_{\mathrm{T50SQR}} + \beta_{\mathrm{AROT90}} Z_{\mathrm{AROT90}} + \cdots \qquad \textbf{Equation 5-4}$$

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]	HI[1]	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				
	OXYSQR	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					
	OXYSQR	T50SQR	T90SQR	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 0 above). 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 $\mathbf{X\beta_{target}}$ **and** $\mathbf{X\beta_{base}}$ for estimates on the target and base fuels, then the ratio difference in emissions is given by Equation 5-5.

$$f_{\text{adj}} = \frac{\exp\left(\mathbf{X\beta}_{\text{target}}\right)}{\exp\left(\mathbf{X\beta}_{\text{base}}\right)} \qquad \textbf{Equation 5-5}$$

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. 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 (EPAct Models: HC, CO, NO_x, PM)

6.1 Introduction: the EPAct 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 (EPAct).

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 "EPAct/V2/E-89" program (or "EPAct"), 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 to represent the latest technologies on the market at the time the program was launched in 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 EPAct 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. (5^{th} to 95^{th} percentiles for each property).

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

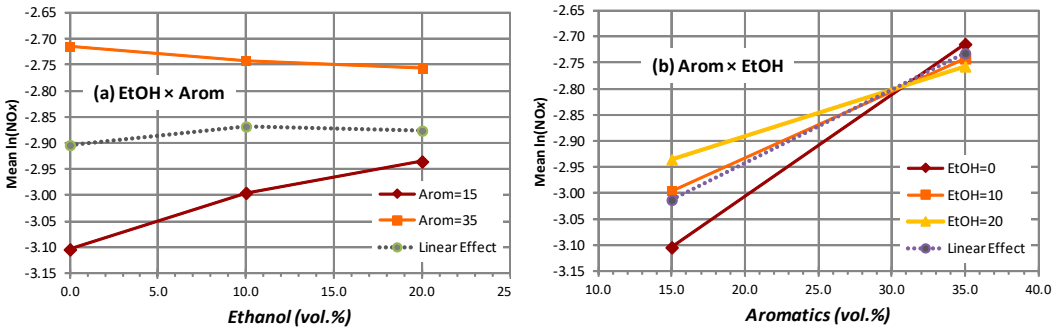
$$Y = \beta_0 + \beta_1 \text{etOH} + \beta_2 \text{Arom} + \beta_3 \text{RVP} + \beta_4 \text{T50} + \beta_5 \text{T90} + \beta_6 \text{T50}^2 + \beta_{11} \text{etOH}^2 \beta_7 \text{etOH} \times \text{Arom} + \beta_8 \text{etOH} \times \text{RVP} + \beta_9 \text{etOH} \times \text{T50} + \beta_{10} \text{etOH} \times \text{T90} + \varepsilon$$

Equation 6-1

In the equation, the linear terms (e.g., $\beta_1$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 etOH×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 lnNO_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 lnNO_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 EPAct 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 (CO_2), carbon monoxide (CO), total hydrocarbons (THC), methane (CH_4), 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 EPAct exhaust research program and analysis are extensively documented in the "EPAct Test Program Report" [41] and "EPAct Analysis Report."[42] This chapter describes how the statistical models developed during the EPAct study are applied in the MOVES model.

Table 6-3. Measured Parameters for Fuels in the Phase-3 EPAct 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]

$$Z_i = \frac{x_i - \bar{x}}{s} \qquad \textbf{Equation 6-2}$$

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.

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

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 $ZZ_{\text{etOH×etOH}}$, 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.

$$ZZ_{\text{etOH×etOH}} = \frac{Z_{\text{etOH}}Z_{\text{etOH}} - m_{Z_{\text{etOH}}Z_{\text{etOH}}}}{s_{Z_{\text{etOH}}Z_{\text{etOH}}}} \qquad \textbf{Equation 6-4}$$

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

$$ZZ_{\text{etOH×eArom}} = \frac{Z_{\text{etOH}}Z_{\text{Arom}} - m_{Z_{\text{etOH}}Z_{\text{Arom}}}}{s_{Z_{\text{etOH}}Z_{\text{Arom}}}} \qquad \textbf{Equation 6-5}$$

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 EPAct 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
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) (Equatiom 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 (ln*Y*), 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.

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

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 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	*Full Model (superset)*					*Reduced Model (SM1)*				
	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_e	0.0555	0.0127	941	4.36	0.00001	0.0548	0.0127	941	4.33	0.00002
Z_a	0.0678	0.0089	941	7.64	0.00000	0.0676	0.0089	941	7.62	0.00000
Z_r	-0.0439	0.0101	941	-4.33	0.00002	-0.0445	0.0101	941	-4.43	0.00001
Z_5	0.1296	0.0128	941	10.14	0.00000	0.1288	0.0127	941	10.15	0.00000
Z_9	0.0178	0.0089	941	2.01	0.04481	0.0183	0.0088	941	2.07	0.03898
ZZ_{ee}	0.0452	0.0171	941	2.64	0.00834	0.0436	0.0168	941	2.60	0.00959
ZZ_{55}	0.0742	0.0128	941	5.80	0.00000	0.0736	0.0128	941	5.77	0.00000
ZZ_{ea}	0.0183	0.0087	941	2.11	0.03542	0.0179	0.0087	941	2.07	0.03857
ZZ_{er}	0.0044	0.0089	941	0.50	0.61726					
ZZ_{e5}	0.0460	0.0183	941	2.51	0.01227	0.0445	0.0181	941	2.46	0.01409
ZZ_{e9}	0.0208	0.0087	941	2.38	0.01729	0.0214	0.0086	941	2.49	0.01294
σ^2_{veh}	0.1325					σ^2_{veh}	0.1325			
σ^2_{τ}	0.06870					σ^2_{τ}	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	*Full Model (superset)*					*Reduced Model (SM3)*				
	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_e	0.0331	0.0120	819	2.77	0.0057	0.0327	0.0120	819	2.73	0.0066
Z_a	-0.0194	0.0093	819	-2.09	0.0370	-0.0195	0.0093	819	-2.10	0.0360
Z_r	-0.0354	0.0106	819	-3.33	0.0009	-0.0355	0.0106	819	-3.36	0.00080
Z_5	0.0476	0.0129	819	3.69	0.0002	0.0501	0.0129	819	3.89	0.0001
Z_9	0.0506	0.0094	819	5.39	0.0000	0.0514	0.0093	819	5.54	0.00000
ZZ_{ee}	-----					-----				
ZZ_{55}	0.0334	0.0094	819	3.55	0.0004	0.0337	0.0094	819	3.59	0.00036
ZZ_{ea}	0.0121	0.0091	819	1.33	0.1839					
ZZ_{er}	-0.0121	0.0092	819	-1.31	0.1914					
ZZ_{e5}	-----					-----				
ZZ_{e9}	-0.0116	0.0092	819	-1.2600	0.2080					
σ^2_{veh}	0.8406					σ^2_{veh}	0.8384			
σ^2_{ε}	0.06669					σ^2_{ε}	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	*Full Model (Superset)*					*Reduced Model (SM1)*				
	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^2_{veh}	0.3917					0.3920				
σ^2_{ε}	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	*Full Model (superset)*					*Reduced Model (SM4)*				
	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^2_{veh}	1.9182					σ^2_{veh}	1.9187			
σ^2_{ε}	0.1250					σ^2_{ε}	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	*Full Model (Superset)*					*Reduced Model (SM2)*				
	Estimate	Std.Err.	d.f.	*t*-value	Pr> *t*	Estimate	Std.Err.	d.f.	*t*-value	Pr> *t*
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^2_{veh}	0.5926					0.5925				
σ^2_{ε}	0.1454					0.1458				

Table 6-11. NO_x (Bag 2): Coefficients and Tests of Effect for the Full and Reduced Models, with BIC = 1118.40 and 1105.17, respectively. Models fit without the Chevrolet Cobalt. Note that the eight terms in the Full Model include those in the top 10 candidate models, as ranked by BIC.

Effect	*Full Model (superset)*					*Reduced Model (SM6)*				
	Estimate	Std. Err.	d.f.	*t* -value	Pr>*t*	Estimate	Std. Err.	d.f.	*t* -value	Pr>*t*
Intercept	-4.5680	0.1844	14	-24.8	0.00000	-4.5692	0.1842	14	-24.8	0.000000
Z_e	0.05813	0.01952	879	2.98	0.0030	0.06299	0.01444	879	4.36	0.000014
Z_a	0.04469	0.01492	879	3.00	0.0028	0.04407	0.01465	879	3.01	0.0027
Z_r	-0.01729	0.01653	879	-1.05	0.30					
Z_5	-0.00245	0.02024	879	-0.12	0.90					
Z_9	0.00491	0.01481	879	0.33	0.74					
ZZ_{ee}	-0.00447	0.01525	879	-0.29	0.77					
ZZ_{55}	---	---	---	---	---	---	---	---	---	---
ZZ_{ea}	0.00478	0.01455	879	0.33	0.74					
ZZ_{er}	0.01418	0.01455	879	0.97	0.33					
ZZ_{e5}	---	---	---	---	---	---	---	---	---	---
ZZ_{e9}	---	---	---	---	---	---	---	---	---	---
σ^2_{veh}	0.4730					σ^2_{veh}	0.4720			
σ^2_{ε}	0.1830					σ^2_{ε}	0.1836			

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

Effect	*Full Model*					*Reduced Model (FM6)*				
	Estimate	Std. Err.	d.f.	χ^2- value	Pr>χ^2	Estimate	Std. Err.	d.f.	χ^2- value	Pr>χ^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^2_{veh} [1]						0.4251				
σ^2_{ε}	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	*Full Model*					*Reduced Model (FM8)*				
	Estimate	Std. Err.	d.f.	χ^2- value	Pr>χ^2	Estimate	Std. Err.	d.f.	χ^2- value	Pr>χ^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^2_{veh} [1]						0.7827				
σ^2_{ε}	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) and E85 (fuelTypeID = 5). The adjustments described in this document are applied to gasoline blends containing 0-15 vol.% ethanol and high-level ethanol blends containing 70 vol.% or more ethanol.

Engine technology: For MOVES, these adjustments 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
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: MOVES 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 De-standardization of Model Coefficients

As described above in 6.2.1, the values for the fuel property predictors are 'standardized' before fitting the models. In MOVES2014, the expressions used to calculate the fuel adjustments have included the standardization of fuel properties for base and target fuels. The additional calculations make the corresponding GFRE expressions extremely complicated.

For application of selected models in MOVES3, we have reversed this process to develop sets of "de-standardized" model coefficients. In applying the models, the benefit of de-standardization is that it simplifies the process by enabling the entry of fuel properties in their native units, e.g., vol.%, psi, ◦F, etc. In the MOVES GFRE table, the resulting expressions are shorter, simpler and easier to follow.

6.4.1 De-standardizing Linear Terms

For the simple linear terms, the process is straightforward. We can illustrate an example for the emission y so that the response variable is $\ln y$.

If we include the model intercept and a single linear term, as in Equation 6-7, we see

$$\ln y = \beta_0 + \beta_1 Z \qquad \textbf{Equation 6-7}$$

where as in Equation 6-2, *Z* is the "first-stage" standardized value for the fuel property *x*, for which, if we substitute the definition of *Z* in terms of *x* and its mean and standard deviation, we obtain the expression in Equation 6-8.

$$\ln y = \beta_0 + \beta_1 \left(\frac{x - \bar{x}}{s}\right) \qquad \textbf{Equation 6-8}$$

We can distribute the slope coefficient β_1 and recollect terms to obtain Equation 6-9,

$$\ln y = \beta_0 + \frac{\beta_1 x}{s} - \frac{\beta_1 \bar{x}}{s} \qquad \textbf{Equation 6-9}$$

which we can rearrange to show the modified slope and intercept terms, i.e., the de-standardized slope term is simply β_1/s, as shown in Equation 6-10.

$$y = \left(\beta_0 - \frac{\beta_1 \bar{x}}{s}\right) + \frac{\beta_1 x}{s} \qquad \textbf{Equation 6-10}$$

6.4.2 De-standardizing 2nd-order Terms

For interaction terms, involving "second-stage" standardized terms, the process is similar but more detailed. We'll consider an example of an interaction term between fuel properties 1 and 2, in which "1" would be ethanol and the other could be any of the other four fuel properties, e.g., aromatics, RVP, T50 or T90. These terms are denoted by the notation 'ZZ_{12}.' In model fitting, we respected 'hierarchy,' meaning that if the term ZZ_{12} was included in the model, both linear terms Z_1 and Z_2 were also included, as shown in Equation 6-11.

$$\ln y = \beta_0 + \beta_1 Z_1 + \beta_2 Z_2 + \beta_{12} ZZ_{12} \qquad \textbf{Equation 6-11}$$

The two linear terms would be de-standardized as shown above. Limiting attention to the interaction term, Equation 6-12 shows the 'second-stage' standardized term as constructed from the 'first-stage' terms for the two predictors.

$$\beta_{12} ZZ_{12} = \beta_{12} \left(\frac{Z_1 Z_2 - m_{12}}{s_{12}}\right) \qquad \textbf{Equation 6-12}$$

In this expression, m_{12} and s_{12} are the mean and standard deviation of the product Z_1Z_2 across the fuel set, as shown in Equation 6-5 (page 68). Disassembling the 'first-stage' terms yields Equation 6-13, and

$$\beta_{12}\left(\frac{Z_1Z_2 - m_{12}}{s_{12}}\right) = \beta_{12}\left(\frac{\left(\frac{x_1 - \bar{x}_1}{s_1}\right)\left(\frac{x_2 - \bar{x}_2}{s_2}\right) - m_{12}}{s_{12}}\right) \qquad \textbf{Equation 6-13}$$

distributing across terms in the numerator gives the expression in Equation 6-14.

$$\beta_{12}\left(\frac{\left(\frac{x_1}{s_1} - \frac{\bar{x}_1}{s_1}\right)\left(\frac{x_2}{s_2} - \frac{\bar{x}_2}{s_2}\right) - m_{12}}{s_{12}}\right) \qquad \textbf{Equation 6-14}$$

Multiplying through and rearranging gives Equation 6-15.

$$\beta_{12}\left(\frac{1}{s_{12}}\right)\left(\left(\frac{x_1x_2}{s_1s_2} - \frac{x_1\bar{x}_2}{s_1s_2} - \frac{x_2\bar{x}_1}{s_1s_2} + \frac{\bar{x}_2\bar{x}_1}{s_1s_2}\right) - m_{12}\right) \qquad \textbf{Equation 6-15}$$

In the final step, we can distribute through to obtain the final set of terms shown in Equation 6-16.

$$\frac{\beta_{12}x_1x_2}{s_1s_2s_{12}} - \frac{\beta_{12}x_1\bar{x}_2}{s_1s_2s_{12}} - \frac{\beta_{12}x_2\bar{x}_1}{s_1s_2s_{12}} + \frac{\beta_{12}\bar{x}_2\bar{x}_1}{s_1s_2s_{12}} - \frac{\beta_{12}m_{12}}{s_{12}} \qquad \textbf{Equation 6-16}$$

In this final degree of separation, the individual terms can be applied as appropriate. The first term represents the de-standardized coefficient for the interaction slope term x_1x_2. The second term modifies the slope term for the first fuel property x_1. The third term modifies the slope term for the second fuel property x_2. The fourth and fifth terms, including only constants, modify the intercept term for the model. Note that in applying these terms, the signs of each must be maintained. Thus, signs for the first and fourth terms are positive, and those for the second, third and fifth terms are negative.

The process described above is repeated for the additional interaction terms x_1x_3, x_1x_4 and x_1x_5.

Additionally, the models can contain up to two quadratic terms, such as x_1^2, denoted in the EPAct models as ZZ_{11} and paired with coefficient β_{11}. The process of de-standardizing a quadratic term is a more specific case of de-standardizing an interaction term, i.e., the predictor has an 'interaction' with itself. The final terms for the quadratic for predictor x_1 resolve to the following expression in Equation 6-17.

$$\frac{\beta_{11}x_1^2}{s_1^2 s_{12}} - 2\frac{\beta_{11}x_1\bar{x}_1}{s_1^2 s_{12}} + \frac{\beta_{11}\bar{x}_1^2}{s_1^2 s_{12}} - \frac{\beta_{11}m_{12}}{s_{12}} \qquad \textbf{Equation 6-17}$$

In this final expression, the first term is the de-standardized term for the quadratic term x_1^2. The second term modifies the linear slope term for predictor x_1. As before, the third and fourth terms modify the intercept term for the model.

Sets of standardized coefficients for the models for THC, CO, NO_x and PM have been presented above in Table 6-6 through Table 6-13. Corresponding de-standardized coefficients are presented in Table 6-15 and Table 6-16.

The de-standardized coefficients are useful *only* for application of the models to generate predictions. We need to emphasize that they are *not useful* for interpretation or comparison. As the de-standardized coefficients are expressed in original units for the respective fuel properties, it is not appropriate to compare coefficients for different properties to assess magnitudes of effects. It is also very important to avoid interpreting any individual coefficient as the "effect" of a fuel property. As with the standardized coefficients, it is critical that ensembles of coefficients containing the same predictor must be taken as packages, never individually. Note that the two variance terms for the models are not affected by the process, as the de-standardization involves only manipulation of the coefficients, as described above.

Table 6-15. De-standardized Models representing "Cold-start" Emissions for the Regulated Pollutants.

Model term	THC	CO	NO_x	PM
Intercept	3.4101	9.0464	-3.6914	-0.2078
etOH (v.%)	-0.1120	-0.17827	0.01643	0.02008
Arom (v.%)	0.00435	-0.00403	0.01654	0.03827
RVP (psi)	-0.02763	-0.01770	---	---
T50 (°F)	-0.04460	-0.04129	0.00167	-0.05707
T90 (°F)	-0.00054	-0.00806	---	0.01501
etOH × etOH	0.00087	0.00147	---	---
T50 × T50	0.00012	0.00009	---	0.00015
etOH × Arom	0.00023	0.00027	-0.00031	---
etOH × RVP	---	0.00126	---	---
etOH × T50	0.00026	0.00061	---	---
etOH × T90	0.00014	---	---	---
Vehicle variance	0.1325	0.3920	0.5925	0.4251
Residual error	0.06872	0.07214	0.1458	1.0359

Table 6-16. De-standardized Models representing "Hot-running" Emissions for the Regulated Pollutants.

Model term	THC	CO	NO_x	PM
Intercept	-3.6528	-2.6790	-4.7644	-3.6473
Ethanol (v.%)	0.00415	---	0.00799	0.01429
Aromatics (v.%)	-0.00195	0.00911	0.00440	0.01659
RVP (psi)	-0.02205	0.01855	---	---
T50 (°F)	-0.01953	0.00091	---	---
T90 (°F)	0.00264	0.00226	---	0.00550
etOH × etOH	---	---	---	---
T50 × T50	0.000056	---	---	---
etOH × Arom	---	---	---	---
etOH × RVP	---	---	---	---
etOH × T50	---	---	---	---
etOH × T90	---	---	---	---
Vehicle variance	0.8384	1.9187	0.4720	0.7827
Residual error	0.06717	0.1256	0.1836	1.1337

6.5 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.[8] The base rates are assumed to represent emissions on a "base fuel" which are adjusted by a ratio 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 EPAct study results to derive fuel adjustments for the subsets of vehicles and model years described above.

The models generated using EPAct 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 EPAct exhaust data follow the general structure shown in Equation 6-18 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 $Z_{etOH\times Arom}$ denotes a "standardized" etOH×Arom interaction term. Finally, the term s_ε^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 "$\mathbf{X\beta}$."

$$\text{Emissions (g/mi)} = \exp\left(\beta_0 + \beta_{\text{etOH}} Z_{\text{etOH}} + \beta_{\text{Arom}} Z_{\text{Arom}} + \beta_{\text{T50}} Z_{\text{T50}} + \beta_{\text{etOH}\times\text{Arom}} Z_{\text{etOH}\times\text{Arom}} + 0.5 s_\varepsilon^2\right) = \exp(\mathbf{X\beta}) \qquad \textbf{Equation 6-18}$$

The equivalent expression of the same model using "de-standardized" coefficients, denoted as β^d, with fuel properties x in their respective units is shown in Equation 6-19.

$$\textbf{Emissions (g/mi)} = \exp\left(\boldsymbol{\beta}_0^d + \boldsymbol{\beta}_{\text{etOH}}^d \boldsymbol{x}_{\text{etOH}} + \boldsymbol{\beta}_{\text{Arom}}^d \boldsymbol{x}_{\text{Arom}} + \boldsymbol{\beta}_{\text{T50}}^d \boldsymbol{x}_{\text{T50}} + \boldsymbol{\beta}_{\text{etOH}\times\text{Arom}}^d \boldsymbol{x}_{\text{etOH}\times\text{Arom}} + \mathbf{0.5} s_\varepsilon^2\right) = \boldsymbol{exp}\left(\mathbf{X}\boldsymbol{\beta}^d\right) \qquad \textbf{Equation 6-19}$$

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 6-20. Please note that this calculation does not pull the base fuel characteristics from the *baseFuels* database table; instead, the base fuel properties are directly included in the equations in the *GeneralFuelRatioExpression* database table.

$$\text{Fuel Effect} = \frac{\exp\left(\mathbf{X\beta}_{\text{in-use}}^{\boldsymbol{d}}\right)}{\exp\left(\mathbf{X\beta}_{\text{base}}^{\boldsymbol{d}}\right)} = \exp\left(\mathbf{X\beta}_{\text{in-use}}^{\boldsymbol{d}} - \mathbf{X\beta}_{\text{base}}^{\boldsymbol{d}}\right) \qquad \textbf{Equation 6-20}$$

The sets of de-standardized coefficients for four individual pollutants, including THC, CO, NO_x, and PM have been presented in Table 6-15 and Table 6-16 above. These models are applied in MOVES through the *GeneralFuelRatioExpression* table, described in detail in Section 6.6.

The table includes two sets of coefficients for each pollutant, representing the effects of the fuel properties on start and running exhaust emissions, respectively.[f] In some cases, the 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.

[f] For all models, "start" and "running" emissions are represented by results measured on Bags 1 and 2 of the LA92 cycle, respectively.

The coefficients can be understood as the change in the natural logarithm of emissions (e.g., ΔlnCO) associated with a change in the fuel property of 1.0 units, and assuming that *the other fuel properties remain constant*.

6.6 The Database Table "GeneralFuelRatioExpression"

A detailed description of the "generalFuelRatioExpression" table is shown below in Table 6-17.

Table 6-17. 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., 2060
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.	

6.6.1 Examples

We show an example 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. The entire expression for NO_x starts is shown below in Table 6-18. Due to its length, the whole is divided into terms and segments, which, along with descriptions, are presented in Table 6-19.

Table 6-18. 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, reid vapor pressure, T50, T90 and sulfur).

if(sulfurLevel>30,((exp(-3.69135462091143-0.000306740025914599*ETOHVolume*aromaticContent+0.0164283073605751*ETOHVolume+0.0165361679107306*aromaticContent+0.0016732745247391 2*T50))*(1+(0.425*((exp(0.351*ln(303))-exp(0.351*ln(30)))/exp(0.351*ln(30)))+(1.0-0.425)*(1.47*(exp(0.351*ln(sulfurLevel))-exp(0.351*ln(30)))/(exp(0.351*ln(30)))))))/(0.05932198247482521*1.53198632575613),((exp(-3.69135462091143-0.000306740025914599*ETOHVolume*aromaticContent+0.0164283073605751*ETOHVolume+0.0165361679107306*aromaticContent+0.0016732745247391 2*T50))/0.05932198247482521)*(1.0-0*(30-sulfurLevel)))

Table 6-19. Expression stored in the Field "fuelEffectRatioExpression" in the Table "GeneralFuelRatioExpression," illustrating the combined application of non-sulfur and sulfur fuel adjustments for start NO_x emissions.

if(sulfurLevel>30,	Initiate condition to be applied for sulfur level > 30 ppm
(exp(-3.69135462091143	Initiate exponential expression, enter intercept for EPAct model.
-0.000306740025914599*ETOHVolume*aromaticContent	enter interaction term for ethanol×aromatics
+0.0164283073605751*ETOHVolume	enter linear term for etahanol
+0.0165361679107306*aromaticContent	enter linear term for aromatics
+0.0016732745247391 2*T50))	enter linear term for T50, close exponential term
(1+(0.425((exp(0.351*ln(303))-exp(0.351*ln(30)))/exp(0.351*ln(30)))+(1.0-0.425)*(1.47*(exp(0.351*ln(sulfurLevel))-exp(0.351*ln(30)))/(exp(0.351*ln(30))))))	enter expression to calculate sulfur effect (application of M6Sulf model).
,	Initiate condition for sulfur level ≤ 30 ppm (NOTE: following comma, condition is implicit).
(exp(-3.69135462091143	Initiate exponential expression, enter intercept for EPAct model.
-0.000306740025914599*ETOHVolume*aromaticContent	enter interaction term for ethanol×aromatics
+0.0164283073605751*ETOHVolume	enter linear term for etahanol
+0.0165361679107306*aromaticContent	enter linear term for aromatics
+0.0016732745247391 2*T50))	enter linear term for T50, close exponential term
/0.05932198247482521)	enter ratio to emissions on base fuel
(1.0-0(30-sulfurLevel)))	enter expression to estmate sulfur effect (T2 sulfur model).

Table 6-20 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, using the de-standardized coefficients as presented in Section 6.4. 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 start and running rates represent aggregate results on Bags 1 and 2 of the LA92 cycle, respectively.

For NO_x, the calculations predict decreases of approximately 6% and 1.4% for start and running emissions, respectively. For THC, corresponding reductions for start and running emissions are 11% and 3.3%, respectively, as shown in Table 6-21.

Table 6-20. NO_x: Application of Models for Tier 3 Certification Fuel and a MOVES Base Fuel, with Calculation of Fuel Adjustments.

Fuel properties **Models**

Property	Fuel		Coefficients	
	base	T3	Start	Running
etOH (vol.%)	10	9.8	0.01643	0.00799
Arom (vol.%)	25.77	23	0.01654	0.0044
RVP (psi)	8.8	8.95	0	0
T50 (°F)	212.3	200	0.00167	0
T90 (°F)	321.7	325	0	0
etOH × etOH	100	96.04	0	0
T50 × T50	45,071	40,000	0	0
etOH × Arom	257.7	225.4	-0.00031	0
etOH × RVP	88	87.71	0	0
etOH × T50	2123	1960	0	0
etOH × T90	3217	3185	0	0
Intercept	1	1	-3.6914	-4.7644
Variance			0.7383	0.6556

Results: start model

ln(NOx)	-2.8262	-2.886
NOx (g/mi)	0.08569	0.08073
Adjustment	1.000	0.942

Results: running model

ln(NOx)	-4.571	-4.585
NOx (g/mi)	0.01436	0.01416
Adjustment	1.000	0.986

Table 6-21. THC: Application of Models for Tier 3 Certification Fuel and a MOVES Base Fuel, with Calculation of Fuel Adjustments.

Fuel properties			Models	
Property	Fuel		Coefficients	
	base	T3	Start	Running
etOH (vol.%)	10	9.8	-0.112	0.00415
Arom (vol.%)	25.77	23	0.00435	-0.00195
RVP (psi)	8.8	8.95	-0.02763	-0.02205
T50 (°F)	212.3	200	-0.0446	-0.01953
T90 (°F)	321.7	325	-0.00054	0.00264
etOH × etOH	100	96.04	0.00087	0
T50 × T50	45,071	40,000	0.00012	0.000056
etOH × Arom	257.7	225.4	0.00023	0
etOH × RVP	88	87.71	0	0
etOH × T50	2123	1960	0.00026	0
etOH × T90	3217	3185	0.00014	0
Intercept	1	1	3.4101	-3.6528
Variance			0.20122	0.90557

Results: start model

ln(THC)	-0.9261	-1.039
THC (g/mi)	0.43804	0.39112
Adjustment	1.000	0.893

Results: running model

ln(THC)	-4.629	-4.662
THC (g/mi)	0.01536	0.01485
Adjustment	1.000	0.967

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 (EPAct),[48] its implementation in the Renewable Fuel Standard (RFS)[49] and passage of the Energy Independence and Security Act of 2007 (EISA).[50] To be consistent with these policies, calendar year 2010 is the first year that E85 usage is modeled and included in the default MOVES database (see Section 7.3).[3] 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.[51,52,53]

In MOVES, the "ethanol (E-85)" category includes fuels containing 70% or more ethanol by volume. MOVES allows E85 use for the following sourcetypes only: passenger cars, passenger trucks, and light commercial trucks.[54]

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 MOVES. The MOVES algorithms for estimating the effects of E85 on air toxics[1] and evaporative[2] hydrocarbons are discussed in their respective reports.

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 EPAct Phase 3 program,[55] National Renewable Energy Laboratory (NREL) E40,[56] Coordinating Research Council (CRC) E-80,[57] and the EPA NRMRL Test Program.[58] The details of each program are described below.

Energy Policy Act (EPAct) Program – Phase 3 of the EPAct 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, including a cold-start test similar to the FTP.

Table 7-1. Description of the Vehicles Tested in EPAct 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	EPAct		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.

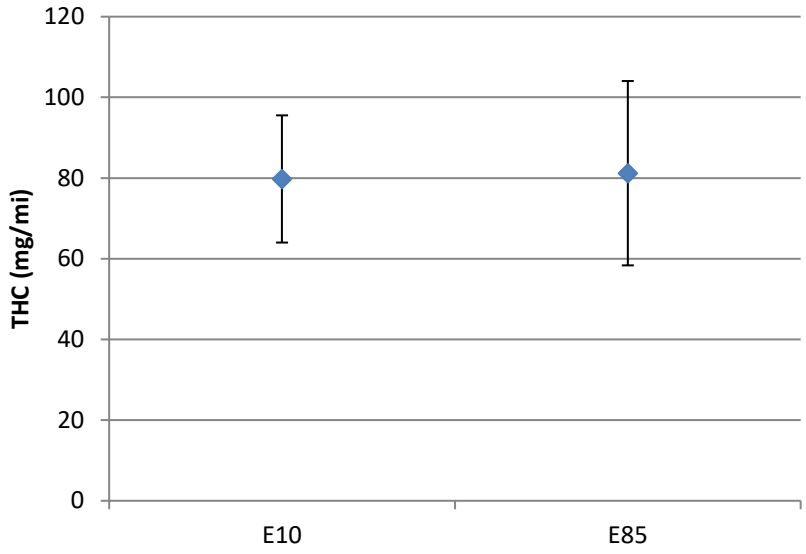


Figure 7-2. Mean NMOG Emissions from Vehicles Running on E10 and E85.

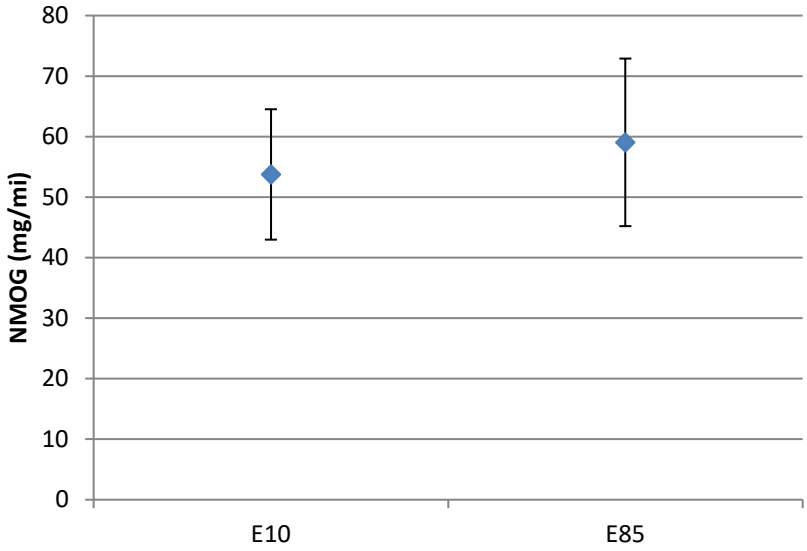


Figure 7-3. Mean NMHC Emissions from Vehicles Running on E10 and E85.

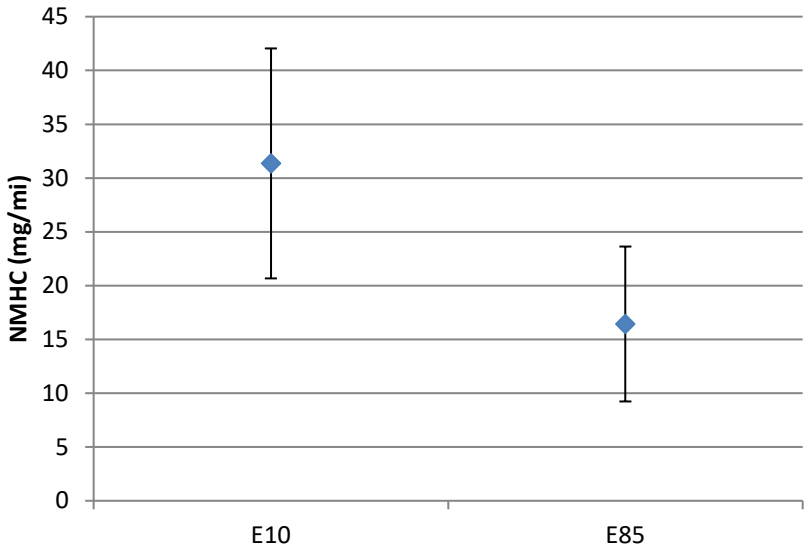


Figure 7-4. Mean CH_4 Emissions from Vehicles Running on E10 and E85.

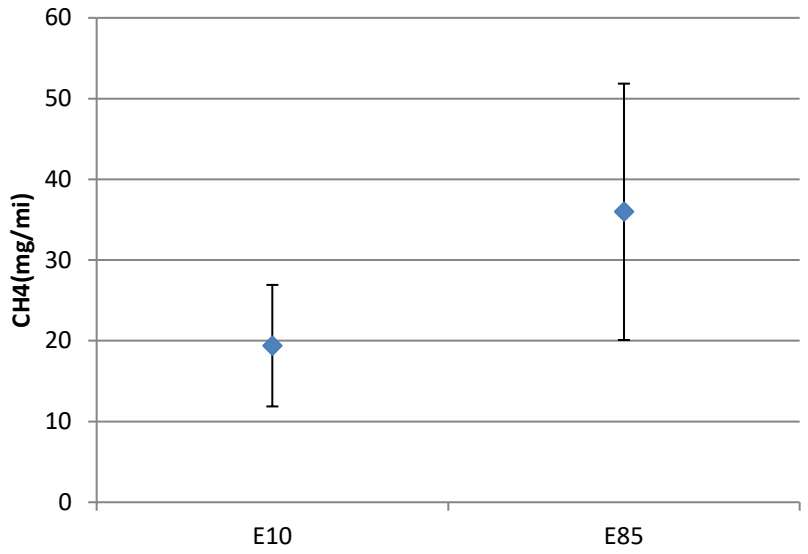


Figure 7-5. Mean NO_x Emissions from Vehicles Running on E10 and E85.

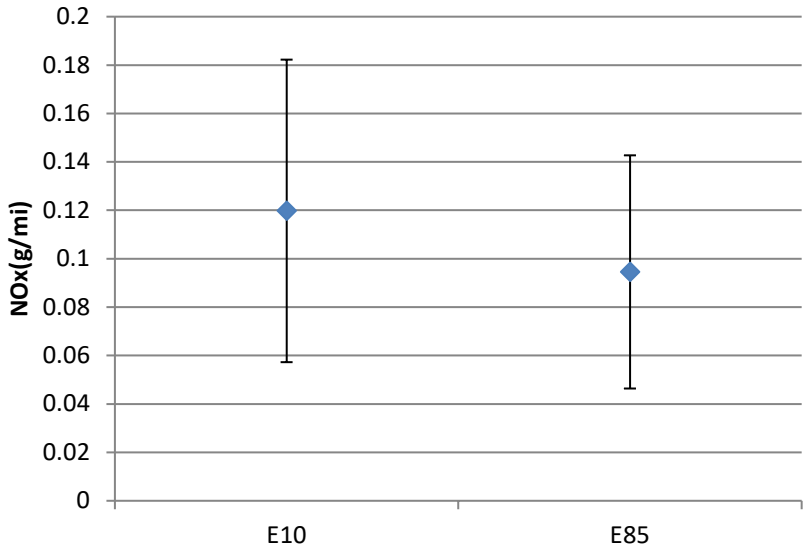


Figure 7-6. Mean $PM_{2.5}$ Emissions from Vehicles Running on E10 and E85.

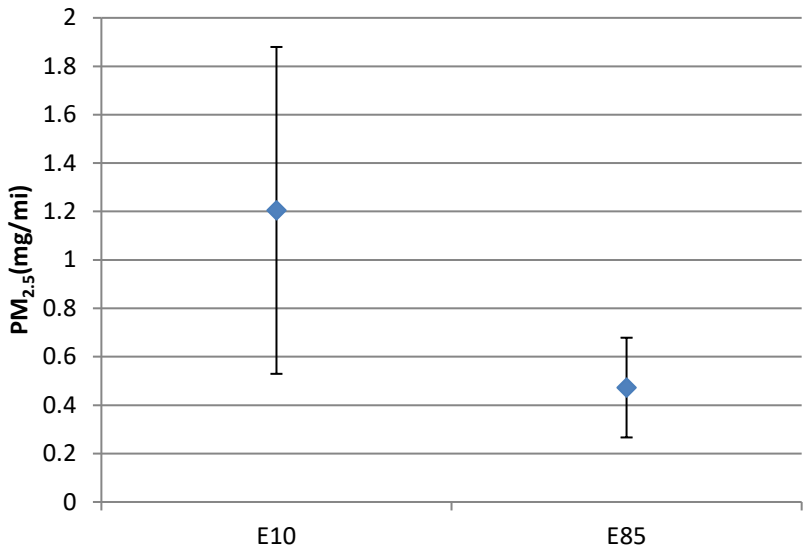
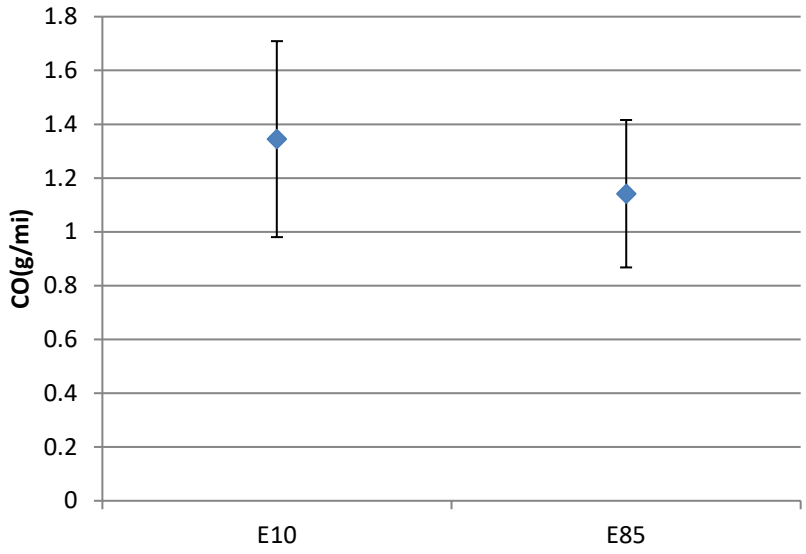


Figure 7-7. Mean CO Emissions from Vehicles Running on E10 and E85.



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 CH_4 emissions showed statistically significant differences between E10 and E85.

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

Pollutant	*p*-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 vehicle regulatory classes capable of running in E85 – light-duty vehicles (LDV) and light-duty trucks (LDT). No fuel adjustments are applied to the pre-2001 MY E85-fueled vehicles.[g] The

[g] MOVES default activity information estimates E85 capable vehicles (flex-fuel vehicles) entered the fleet starting in with model year 1998 vehicles.[54]

Tier 2 fuel effect adjustments equations for gasoline, including the effect of fuel sulfur, are applied to emissions of THC, CO, NO_x, and $PM_{2.5}$ from MY 2001 and later E85-fueled vehicles in passenger cars, passenger trucks, and light commercial trucks source types in the *generalFuelRatioExpression* table (described in Section 6.6).

For E85 fuel effects, MOVES uses fuel properties from both representative E10 fuels and E85 fuels. As shown in Table 7-8, the fuel properties of E10 (e.g., ethanol volume, aromatic content, T50, and T90) are used in estimating E85 fuel effects, instead of directly using E85-specific fuel properties. MOVES uses E10 fuel as the source of these fuel properties for two reasons:

1. Based on our literature review, the emission rates for THC, CO, NO_x, $PM_{2.5}$, NMOG and VOC emissions from E10 and E85-fueled FFVs are not statistically significantly different. By using the E10 fuel properties, MOVES adjusts the E85 vehicle emissions using the same fuel adjustments that are applied to the E10 vehicle emissions.
2. The EPAct fuel program included ethanol volume as a factor in the sample design for ethanol levels only between 0% and 15% by volume. Therefore, the fuel effects based on the EPAct program should not be applied to values of ethanol volume, aromatic content, T50 and T90 from E85 fuels which fall outside of the range of values included in the sample design.

The representative E10 fuel properties used to estimate emissions from E85 fuel-vehicles are stored in the *E10FuelProperties* table by fuel region, calendar year and month for the fuel properties shown in Table 7-8 (except ethanol volume, sulfur level, and benzene content). MOVES sets the ethanol volume to be 10% in the fuel effects equation for E85 in the *generalFuelRatioExpression* table.

RVP is handled differently than the other fuel properties that are used in the EPAct fuel equations. The RVP levels of E85 fuels (Table 7-9) fall approximately within the range of RVP values included in the EPAct sample design (7 and 10 psi, Table 6-2). As such, for estimating THC, CO, NO_x, and $PM_{2.5}$ emissions, MOVES uses the RVP from E85 fuels, which tend to be lower than comparable E10 fuels. For NMOG and VOC emissions, MOVES uses the RVP from E10 as shown in Table 7-8.

Table 7-8. Source of Fuel Properties (E85 or E10) used to Estimate Fuel Effects for MY 2001 and Later E85 Vehicles by Pollutant.

Pollutant	Ethanol Volume	RVP	Sulfur Level	Benzene Content	Aromatic Content	Olefin Content	T50	T90
THC, CO, NO_x, $PM_{2.5}$	E10 (10%)	E85	E85	E85	E10	E10	E10	E10
altTHC[1], altNMHC[1], NMOG, VOC		E10						

Note:
[1] altTHC and altNMHC are the temporary intermediate values from which MOVES calculates NMOG and VOC.

As shown in Table 7-8 and Table 7-9, MOVES uses the sulfur level and benzene content from E85 fuels since the fuel effects for sulfur and benzene content were derived without consideration of the ethanol volume of the fuel. The Tier 2 sulfur model discussed in Section 3.3 has emission adjustments for THC, CO and NO_x emissions. Sulfur level also has an impact on

the sulfate (SO_4, a component of $PM_{2.5}$) and sulfur dioxide (SO_2) as discussed in Section 9. Benzene content influences benzene emissions as discussed in the air toxics report.[1] Therefore, we use the E85-specific sulfur level and benzene content to capture the expected emissions benefit from having lower sulfur and benzene content than comparable E10 fuels.

In summary, MOVES uses the E85 fuel properties for RVP (for THC, CO, NO_x, and $PM_{2.5}$), sulfur level and benzene content from the corresponding E85 fuel assigned to the specific fuel region, calendar year, and month stored in the fuelFormulation table. MOVES currently assumes two distinct E85 fuel formulations for all fuel regions and calendar years[3], with the relevant fuel properties used by MOVES for E85 fuel effects shown in Table 7-9.

Table 7-9. Relevant Fuel Properties used for the E85 Fuel Effects.

E85 Fuel Formulation ID	Month Applied	RVP (psi)	Sulfur Level (ppm)	Benzene Content (% volume)
27001	October through April	10.5	8	0.16%
27002	May through September	7.7		

MOVES uses the olefin content from E10 representative fuels to estimate 1,3-butadiene emissions from E85-fueled vehicles, because E85 fuels have much lower olefin content than the gasoline fuels used to develop the adjustments from the Complex Model. MOVES accounts for the lower 1,3-butadiene emissions in vehicles fueled by E85 compared to E10 using E85/E10 ratios as discussed in the air toxics report.[1]

In MOVES, the estimation of the other organic gas emissions starts with emissions of THC. As discussed above, the THC fuel effects for MY 2001 and later vehicles using E85 are estimated using the fuel properties of E10, with the exception of RVP and sulfur level where E85-specific fuel properties are used. Next, MOVES calculates both methane and NMHC from THC emissions using methane/total hydrocarbon ratios (CH4THCRatio in the database table *methaneTHCRatio*). MOVES applies an E85-specific methane ratio (82% methane for running and 27% for starts) which is directionally consistent with the results shown in Section 7.2, where FFVs fueled with E85 emit higher methane emissions than E10 and correspondingly lower levels of NMHC. The development of the methane/total hydrocarbon ratios for E85-fueled vehicles is documented in the MOVES speciation report.[59]

For calculation of NMOG emissions for model year 2001 and later vehicles using E85, MOVES starts by calculating an intermediate value called "alternative THC (altTHC)" that is never reported to the user. The altTHC value represents THC emissions calculated using the fuel properties from E10 fuels (including RVP), except the sulfur level (Table 7-8). Next, MOVES calculates altNMHC from altTHC using the CH_4/THC ratios from E10-fueled vehicles. Then, MOVES calculates NMOG emissions from the altNMHC emissions using the E10-specific NMOG/NMHC exhaust speciation factors as summarized in Table 7-10. MOVES uses this method because no statistically significant difference was observed in the NMOG emissions rates between E10 and E85-fueled vehicles in Section 7.2.

Although volatile organic compounds (VOC) were not analyzed in Section 7.2, due to a lack of speciated data from the larger study, it was assumed that VOC would behave similarly to NMOG

in terms of response to high-level ethanol fuels for model year 2001 and later FFVs, since the only differences between NMOG and VOC are the presence of ethane and acetone. Therefore, we used the altNMHC emissions and the E10-specific VOC/NMHC speciation ratios to estimate VOC emissions in a similar method as was done for NMOG as summarized in Table 7-10. For a detailed description of the algorithm used to estimate NMOG and VOC emissions from MY 2001 and later E85-fueled vehicles, see Appendix C.

Table 7-10. Calculation of THC, CH_4, NMOG, VOC, and TOG emissions from E85-fueled Vehicles in MOVES

Model Year	THC	CH_4	NMOG	VOC	TOG
1960-2000	E10 base THC rates with no fuel effect adjustments	Calculated from THC emissions using E85 CH_4/THC ratio	Calculated from NMHC emissions using E85 NMOG/NMHC ratios	Calculated from NMHC emissions using E85 VOC/NMHC ratios	NMOG + CH_4
2001-2060	E10 base THC rates with fuel effect adjustments using E10 fuel properties with the exception of RVP and sulfur level from E85	Calculated from THC emissions using E85 CH_4/THC ratios	Calculated from altNMHC emissions using E10 NMOG/NMHC ratios	Calculated from altNMHC emissions using E10 VOC/NMHC ratios	NMOG + CH_4

Because the supporting data for the NMOG comparison in Section 7.2 was based on Tier 2 vehicles, we did not apply the same logic for the pre-2001 MY year vehicles. For those vehicles, we apply the E85-specific speciation factors to calculate NMOG and VOC emissions from the baseline NMHC values as shown in Table 7-10.

7.3.1 Example MOVES Results

Figure 7-8 and Figure 7-9 display the running emission rates (g/mile) for gasoline and E85-fueled light-duty vehicle (LDV) by model year for select pollutants estimated from calendar year 2010 and 2020 national MOVES3 runs. Figure 7-8 through Figure 7-9 display the percent differences between E85 and E10 emission rates by pollutant and model year group for running and start emissions. The percent differences are the same within the outlined model year groups for light-duty vehicles and light-duty trucks.

Figure 7-8 Gasoline and E85-fueled LDV Running Emission Rates (g/mile) by Model Year and Pollutant Estimated from a 2010 MOVES National Run

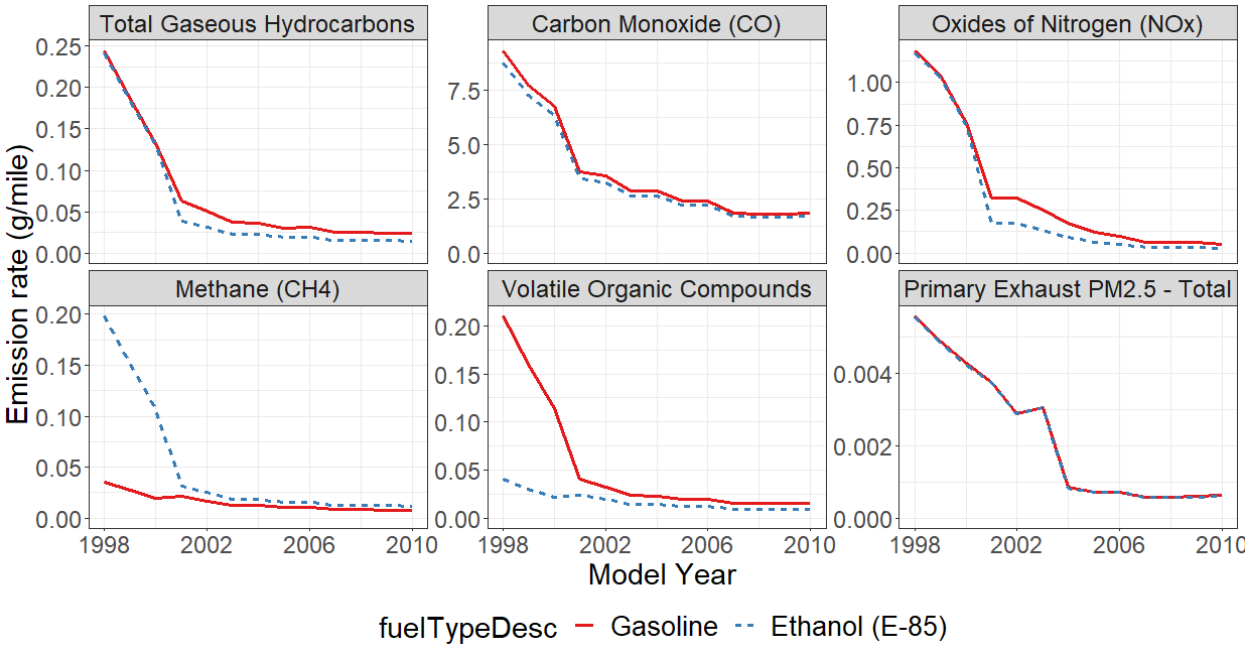
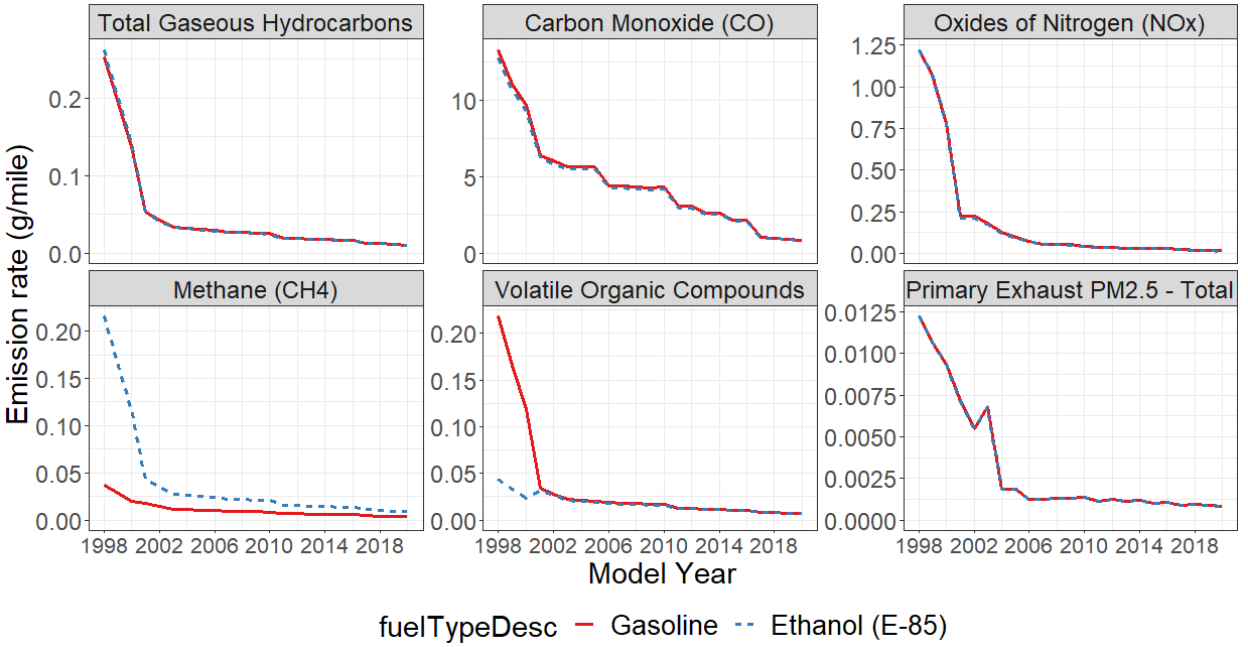


Figure 7-9. Gasoline and E85-fueled LDV Running Emission Rates (g/mile) by Model Year and Pollutant Estimated from a 2020 MOVES National Run



The largest differences in emission rates between gasoline and E85 are due to differences in methane emissions, and the other pollutants which are calculated from methane (NMHC and TOG for all model years, and NMOG and VOC for pre-2001 model years). Methane emissions are significantly higher from E85 vehicles, particularly for the pre-2001 model years, due to the different methane/THC ratios used by MOVES. For example, E85 vehicles use a methane ratio

of 82% in all model years for running exhaust, and E10 vehicles use methane ratio of 15% for pre-2001 model years, and 11% for 2001+ MY vehicles.[59] Significantly higher methane emissions from E85-fueled vehicles compared to gasoline for 2001 and later model year are consistent with the analysis presented in Figure 7-4.

In general, the emission rates for THC, CO, NO_x, VOC and $PM_{2.5}$ emissions from E10 and E85-fueled vehicles are relatively similar to each other across all model years. Because no fuel effects are applied to the pre-2001 model year E85 emission rates, the small observed differences in THC, CO and NO_x emissions are due to the Complex and Predictive Model fuel effects applied to the pre-2001 model year E10-fueled vehicles.

The emission rates of THC, CO, and NO_x for MY 2001+ E85-fueled vehicles are generally lower than the comparable model year E10 emission rates, primarily because of the lower sulfur content and lower RVP properties in E85 fuels compared to E10 fuels. In calendar year 2010, the national average sulfur level for E10 fuels in MOVES is approximately 36 ppm which decreases to 10 ppm by CY 2020. In contrast, the sulfur level of the E85 fuels in MOVES is assumed to be 8 ppm in all years. As such, larger differences in the emission rates are observed between E85 and E10-fueled vehicles in calendar year 2010 (Figure 7-8), when there is a large difference in the sulfur levels. In contrast, when sulfur levels of E85 and 10 fuels are similar (8 ppm and 10 ppm, respectively) in 2020, the emission rates for MY 2001+ vehicles are roughly equivalent for THC, CO, NO_x, VOC and $PM_{2.5}$ (Figure 7-9).

The MY 2001-2016 LDV, and MY 2001-2017 LDT vehicles use the Tier 2 base sulfur level of 30 ppm in the sulfur equation stored in the *generalFuelRatioExpression (GFRE)* table. For MY 2017 and later LDVs and 2018 and later LDTs, the sulfur equations use the Tier 3 base sulfur level of 10 ppm, as described in Section 3.3.4. This change in the base sulfur level explains the small change in the percent differences of E85 and E10 emission rates between the 2001-2016 and 2017-2020 model years for LDV vehicles seen in Figure 7-9.

The $PM_{2.5}$ emission rates are equivalent for the pre-2001 model year vehicles because neither E85 nor gasoline vehicles have fuel effects for these model years, with the exception of sulfate emissions, which are a minor portion of the total $PM_{2.5}$ gasoline emissions. For 2001 and later model years, the emission rates are roughly equivalent for running emissions, because the EPAct $PM_{2.5}$ equation uses the E10 fuel properties to adjust the $PM_{2.5}$ emission rates for both E85 and E10-fueled vehicles. We attribute some of the minor differences between the $PM_{2.5}$ emissions rates of E85 and E10-fueled vehicles for MY 2001 and later vehicles to differences in the fuel properties estimated from the national average of E10 fuel properties and the national average of E10 fuel properties estimated in the E10fuelproperties table.

Emission rates for pollutants that are not adjusted by the equations in the *generalFuelRatioExpression* table, such as CO_2, SO_2, SO_4, are discussed in Section 9.

We recognize that additional data and analysis could improve how vehicles running on high ethanol blends are modeled in MOVES. This could be improved in future versions of MOVES as more data become available.

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 THC 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.[1]

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

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.[60] 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 (2010[60]))

Pollutant Name	Percent Change in Emissions
THC	-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.[61,62]

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 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
THC	-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.

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

To estimate the 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 MOVES3 default fuel supply. The pre-2007 biodiesel factors apply to all diesel tailpipe exhaust processes (running exhaust, start exhaust, extended idle exhaust). The pre-2007 biodiesel factors also apply to all model years (1960-2060) of auxiliary power unit exhaust, because they are projected to have more limited emission controls until 2024.[71] For 2007 and later diesel, the biodiesel fuel adjustment factor for diesel tailpipe exhaust processes is set equal to 0, consistent with the literature review in Section 8.2.

9 Sulfate and Sulfur Dioxide 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 running 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.[63] For diesel engines equipped with catalyzed diesel particulate filters, the sulfate

contribution from lubricating oil can also make up a substantial fraction of the $PM_{2.5}$ exhaust emissions.[64]

Maintaining the capability to model emission changes to fuel sulfur content is important for MOVES. The MOVES particulate emission rates for pre-2004 gasoline and pre-2007 diesel vehicles were derived from sets of measurements on higher fuel-sulfur levels than current fuels; it is thus important that MOVES be able to account for changes in fuel sulfur content in estimating particulate emissions.

In MOVES, sulfate emissions are estimated from $PM_{2.5}$ emissions rather than from fuel consumption. This approach assures that the reference fraction of sulfate is consistent with the $PM_{2.5}$ emissions profile. MOVES also 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 MOVES 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 MOVES algorithm for estimating sulfur dioxides is included in this chapter for consistency. The algorithm for gaseous sulfur-dioxide (SO_2) emissions is based on fuel consumption, but the parameters have been updated in MOVES3 to be consistent with the changes to the $PM_{2.5}$ emission factors.

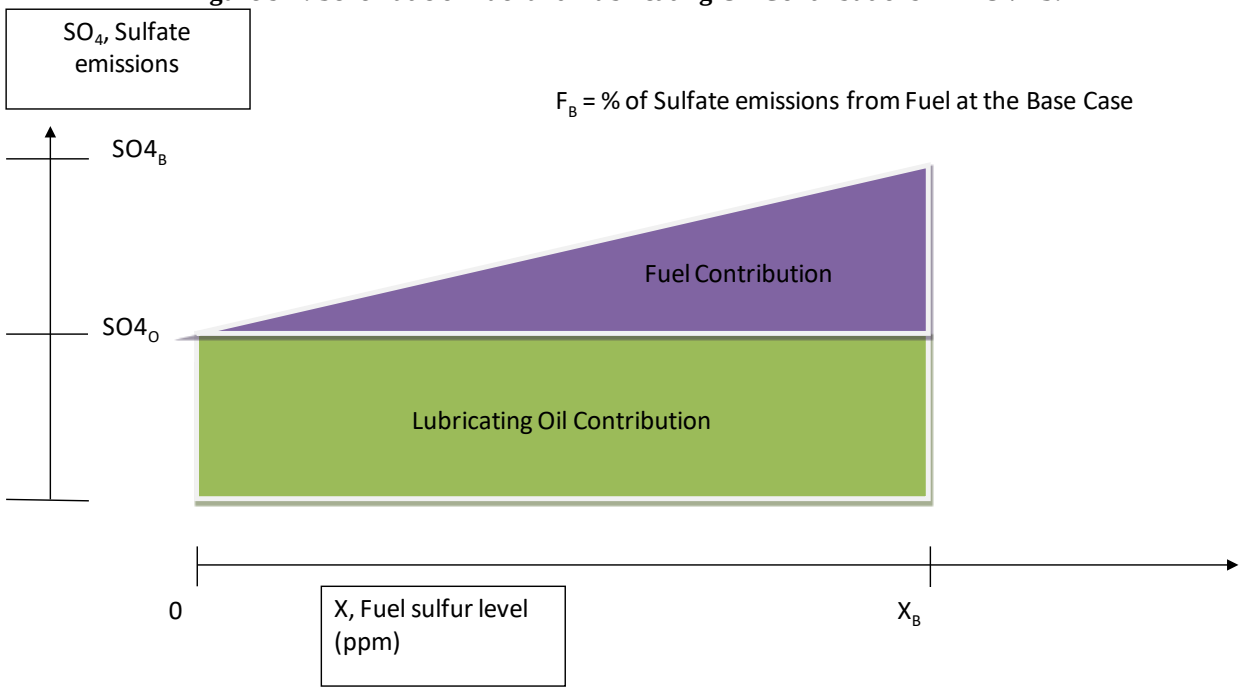
9.2 Sulfate Calculator Summary

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

- Sulfate emissions from the lubricating oil are constant regardless of the fuel sulfur level.
- 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.[65] and Kittelson et al.[63] treated the sulfate contribution from the lubricating oil independently of the fuel sulfur level from diesel engines. Wall et al.[66] demonstrated that sulfate emissions from diesel engines decrease linearly with decreases in the diesel fuel sulfur level down to 100 ppm and 0 ppm. Baranescu[67] and Hochhauser[68] 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.[63] 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 MOVES.



The sulfate calculator uses the concept of reference emission rates and sulfate fractions. MOVES 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 MOVES, the base $PM_{2.5}$ rates are divided between elemental carbon (EC) and the remaining PM that is not elemental carbon (NonECPM). MOVES incorporates these modeling assumptions into Equation 9-1, the derivation of which is included in Appendix A:

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

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 $SO4_x$ = 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 MOVES3 default fuelForumulation and fuelSupply table which specify 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 MOVES3 Speciation report.[59]

Sulfate-bound water (H_2O aerosol) was added in MOVES2014. Currently, the value of $H2O_B$ in MOVES is 0 for all on-road source types, as derived from the $PM_{2.5}$ speciation profiles.[59] If

included in the $PM_{2.5}$ speciation profile, the H_2O aerosol is assumed to be associated with sulfate, and is scaled using the same relationship with fuel sulfur level, as shown in equation:

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

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

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

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)		
Pre-2004 light-duty gasoline and E85 (passenger cars and trucks and light-commercial trucks)	running exhaust	7.2%	8.4%	161.2	68.7%
	start exhaust	0.9%	1.7%		
2004+ light-duty gasoline and E85	running exhaust	Varies by model year[a] (7% to 3%)	8.4%	23.5	24.2%
	start exhaust	Varies by model year[a] (1% to 0.5%)	1.7%		
Motorcycles and heavy-duty gasoline sourcetypes (all model years)	running exhaust	7.2%	8.4%	161.2	68.7%
	start exhaust	0.9%	1.7%		
Pre-2007 diesel (all sourcetypes)	running exhaust	1.0%	4.9%	172.0	72.6%
	start, extended idle and APU	5.3%	9.8%		
2007+ diesel (all sourcetypes)	running, extended idle, start	67.6%	73.6%	11.0	48.3%
Pre-2002 compressed natural gas (all sourcetypes)	running, extended idle, start	0.6%	0.7%	5.0	0.0%
2002+ Compressed natural gas (all sourcetypes)	running, extended idle, start	1.0%	1.2%	5.0	0.0%

[a] The EC/PM fraction varies by model year as discussed in the light-duty exhaust report[8], thus the sulfate/PM fraction also varies by model year.

The following sections discuss 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

9.3.1 Pre-2004 Light-duty Gasoline Vehicles

The reference sulfate fractions and the reference fuel sulfur level for pre-2004 light-duty gasoline vehicles are estimated from the Kansas City Light-Duty Vehicle Emissions Study (KCVES).[37] The use of the KCVES for estimating $PM_{2.5}$ emission rates is documented in the MOVES3 Light-duty Vehicle Emission Rate report,[8] and the derivation of the sulfate emission factor is documented in the TOG and PM Speciation Report.[59] The pre-2004 light-duty gasoline 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.[69] 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 for pre-2004 light-duty gasoline sourceTypes: passenger cars and trucks and light-commercial trucks (sourceTypeID 21,31,32) are displayed in Table 9-2.

Table 9-2. Sulfate Calculator Parameters for 2004+ Light-duty Gasoline Vehicles.

	Kansas City Light-Duty Vehicle Emissions Study (KCVES)	Tier 2 PM update
Model Year Range of Measured Vehicles	1968-2004 (VMT weighted)	2007-2014
Model Year Range Applied in MOVES	1960-2003	2004-2060
Sulfur (ppm) (x_B)	161.2	23.5
Oil Sulfate Contribution (mg/mi)	0.106	0.106
Fuel Sulfate Contribution (mg/mi)	0.233	0.034
Oil Sulfate Contribution %	31.3%	75.8%
Fuel Sulfate Contribution % (F_B)	68.7%	24.2%

9.3.2 2004 and later Light-duty Gasoline Vehicles

We updated the MY 2004 and later light-duty PM emission rates in MOVES3 using data from six different studies as documented in the light-duty vehicle emission rate report[8]. The updated base sulfur level for the MY 2004+ emission rates (calculated by averaging each vehicle test by its associated fuel sulfur level) is 23.5 ppm as shown in Table 9-2.

We also updated the fraction of the fuel sulfate contribution (F_B). Table 9-2 contains the estimated oil and fuel sulfate contributions estimated from the Kansas City Light-Duty Vehicle Emissions Study (KCVES) derived in Appendix A.2. For the Tier 2 PM update, we assumed that the sulfate contribution from lubricating oil is unchanged (0.106 mg/mile), but that the sulfate from the fuel is reduced proportionally to the fuel sulfur level, as consistent with the assumptions used to derive the sulfate calculator in Appendix A, and shown in Equation 9-3.

$$\boldsymbol{Fuel\ Sulfate\ Contribution}_{Tier\ 2} = \boldsymbol{Fuel\ Sulfate\ Contribution}_{KCVES} \times \left(\frac{x_{Tier\ 2}}{x_{KCVES}}\right) = 0.233\ \left(\frac{mg}{mile}\right) \times \left(\frac{23.5\ ppm}{161.2\ ppm}\right) = 0.034\ \left(\frac{mg}{mile}\right) \quad \textbf{Equation 9-3}$$

We then calculated the fuel sulfate fraction, (F_B), by re-calculating the relative sulfate emissions contributed from the lubricating oil and the gasoline using Equation 9-4. We estimate that the gasoline fuel contributes to less than a quarter of the sulfate emissions from 2004 and later vehicles, while the gasoline fuel contributes to over two-thirds of sulfate emissions estimated from 2003 and earlier model year vehicles as shown in Table 9-2.

$$F_{B\ Tier\ 2} = \left(\frac{Sulfate\ from\ fuel}{Sulfate\ from\ oil\ and\ fuel}\right) = \left(\frac{0.034}{0.106 + 0.034}\right) = 24.2\% \quad \textbf{Equation 9-4}$$

The 2004 and later model year emission rates have updated fractions of elemental carbon to particulate matter (EC/PM), which vary by model year according to the fraction of port-fuel injection (PFI) and gasoline direct injection (GDI) vehicles.[8] Despite the updated elemental carbon fractions, we continue to use the same $PM_{2.5}$ speciation profile[59] derived from the KCVES to estimate the components of the non-elemental carbon particulate matter (nonECPM) for all model year gasoline vehicles. As such, we continue to apply the same reference sulfate fraction, SO_4/NonECPM (S_B), derived from the KCVES, to the 2004 and later model year gasoline vehicles. Because the EC/PM fraction varies by model year for the 2004 and later vehicles, the sulfate/PM fraction also varies for the 2004+ model year vehicles as noted in Table 9-1.

9.3.3 High Ethanol Blend (E85) Gasoline Vehicles

The sulfate values derived for light-duty gasoline vehicles are also applied to flex-fuel vehicles fueled on E85. Flex-fuel vehicles use the same emission rates, EC/PM fractions and speciation fractions as light-duty gasoline vehicles. Because E85 has lower sulfur content than gasoline, the E85-fueled vehicles are estimated to have lower sulfate emissions compared to those fueled with gasoline.

9.3.4 Motorcycles Heavy-duty Gasoline Vehicles

The sulfate values derived for pre-2004 light-duty gasoline vehicles are also applied to all model years of the other gasoline-sourcetypes including motorcycles, heavy-duty gasoline trucks and gasoline-powered buses (sourceTypeID 11, 42, 43, 52, 52, 53, 54, and 61). These sourcetypes also use the same EC/PM fractions[71] and PM speciation profiles[59] derived from the Kansas City Light-duty Vehicle Emissions Study. In MOVES3, we have updated the 2010 and later HD $PM_{2.5}$ emission rates for gasoline vehicle to be set equal to heavy-duty diesel $PM_{2.5}$ emission rates. However, we have not updated the gasoline PM speciation data, and we continue to assume that the $PM_{2.5}$ rates are still based on a 161.2 ppm sulfur fuel.

9.4 Diesel Vehicles

9.4.1 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).[70] The E55/59 study is also used to derive the $PM_{2.5}$ emission rates for medium- and heavy-duty diesel in MOVES3.[71] 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[h].

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.[72] The DECSE project was conducted to investigate the impact of low-sulfur diesel fuel standards on diesel emissions. Specifically, the DESCE conducted testing of two engines at four sulfur

[h] See Table 11 in Clark et al.[70]

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 MOVES. 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.

9.4.2 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.[63] 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 because it is the sulfur level of the reference conventional low-sulfur diesel (fuelFormulationID 20) in MOVES3. 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.[73] 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).[74] 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 MOVES3 is based on data acquired from these four engines. The fuel-sulfur level tested in the ACES program is 4.5 ppm.[63] 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 $SO_4/PM_{2.5}$ 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 MOVES3 as shown in Table 9-1. Additional details on the analysis are included in Appendix A.4.

9.5 Compressed Natural Gas

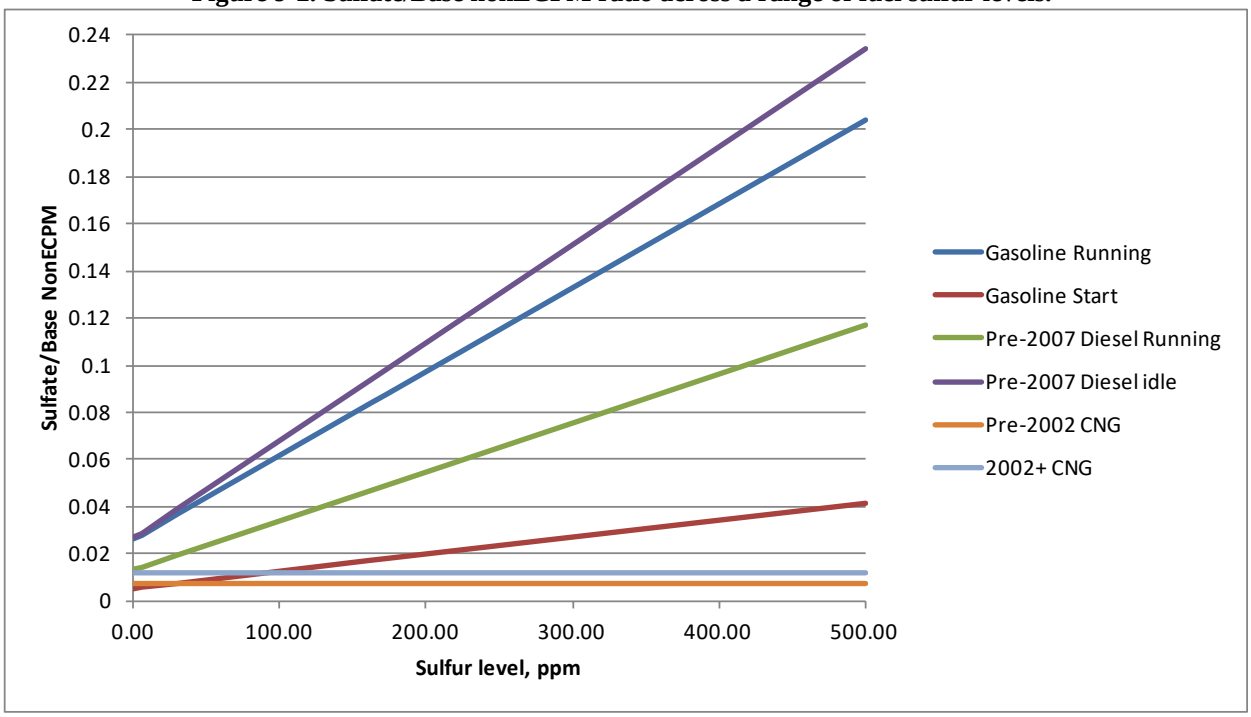
We had limited data on sulfate emissions from engines running on compressed natural gas, especially regarding the relative contribution of the lubricating oil and CNG fuel to sulfate emissions. As such, we do not adjust the sulfate emissions according to fuel sulfur level. We derived a constant fraction 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.[59] We set F_B coefficient to 0, so that MOVES estimates the same sulfate emissions regardless of the sulfur level in the CNG fuel.

9.6 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 ratio 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 pre-2004 gasoline passenger cars, heavy-duty diesel long-haul combination trucks, and CNG transit bus emissions estimated using MOVES2014[i] for a state-wide (Michigan) run in calendar year 2011.

The base nonECPM emission rates in MOVES for pre-2007 MY 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)]. For diesel sulfur level of 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

[i] While the intercept (0 ppm) values are updated in MOVES3 with the updated $PM_{2.5}$ emission rates, the adjustments to the sulfate emission rate according to the fuel sulfur level shown in this analysis are unchanged from MOVES2014.

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 pre-2004 model year 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) in calendar year 2011 estimated using national default data in MOVES2014.

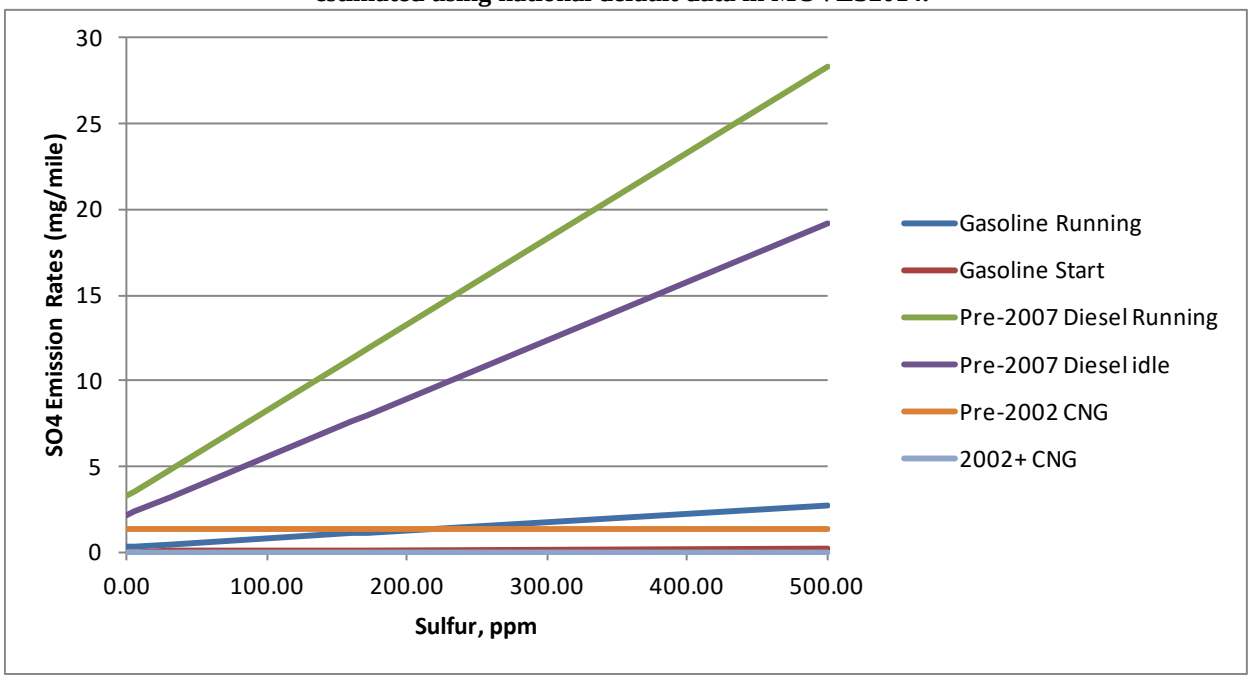
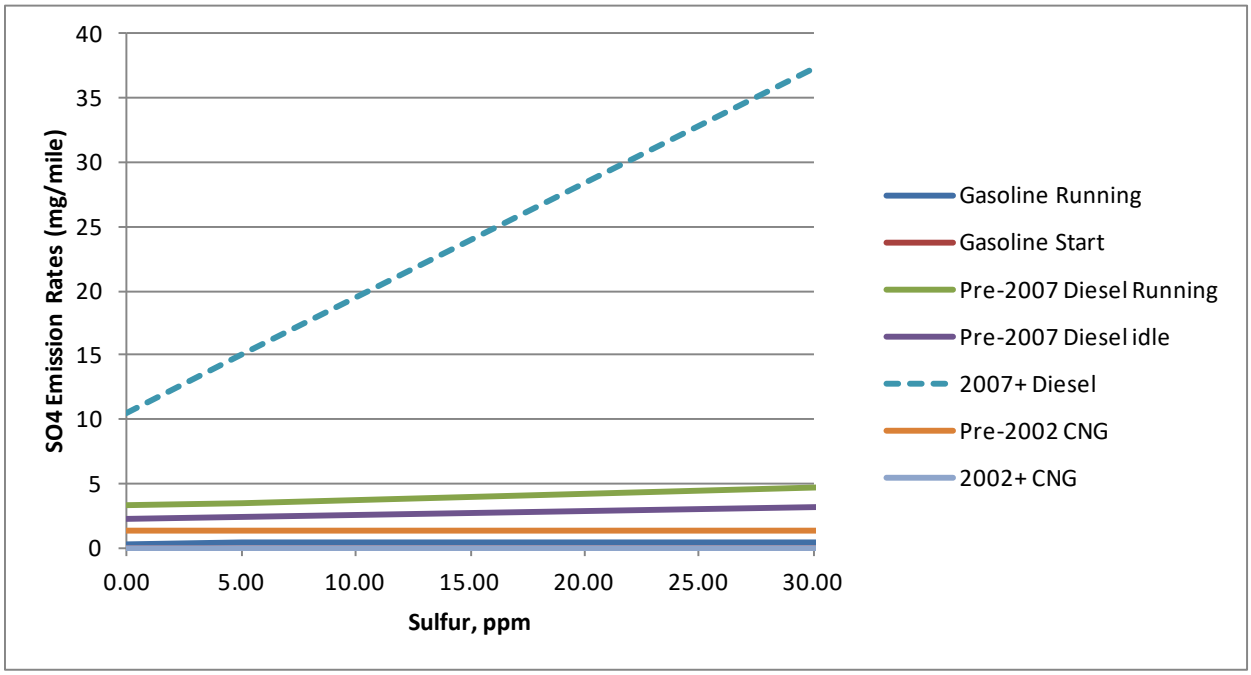


Figure 9-4 plots the estimated sulfate emissions (including 2007+ diesel engines) across a smaller range of fuel sulfur levels (0 to 30 ppm). The 2007+ diesel engines clearly have the largest sulfate emission rates (mg/mile) across all sulfur levels, and also have the largest sensitivity to fuel sulfur 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 (from running, start, and idle processes). 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 nonECPM 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) in calendar year 2011 estimated using national default data in MOVES2014.



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

9.7 Sulfur Dioxide Emissions Calculator

The MOVES SO_2 algorithm calculates SO_2 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 SO_2 calculator assumes that all of the sulfur in SO_2 emissions originate from the fuel. This assumption is reasonable because most of the sulfur originates from the fuel on a mass-balance basis, 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.[63]

SO_2 emissions are calculated using Equation 9-5:

$$\boldsymbol{SO_2(g) = FC(g) \times [S]\,(ppm) \times \frac{MW_SO_2}{MW_S} \times fSO_2 \times \left(\frac{10^{-6}}{ppm}\right)} \qquad \textbf{Equation 9-5}$$

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 9-6.

$$\frac{MW\ SO_2}{MW\ S} = \frac{32 + (2 \times 16)\frac{\mathbf{g}}{\mathbf{mol}}}{32\frac{\mathbf{g}}{\mathbf{mol}}} = \mathbf{2.0} \qquad \textbf{Equation 9-6}$$

fSO_2 = Fraction of fuel sulfur that is converted to gaseous SO_2 emissions. The SO_2 conversion fraction is calculated as the fraction of fuel sulfur not converted to sulfate.

In MOVES3, the SO_2 calculator first calculates the product of $FC(g) \times [S]\ (ppm)$. Then, it multiplies the product by the SO_2 emission factor which combines the last three terms of Equation 9-5 including the ratio of molecular masses Equation 9-6.

The SO_2 conversion values and resulting SO_2 emission factors for use in MOVES3 are displayed in Table 9-3 and stored in the *sulfateemissionrate* table.[j]

Table 9-3. SO_2 conversion efficiencies and MOVES SO_2 emission factors.

Source	SO_2 conversion efficiency (%)	SO_2 EF (1/ppm)
Gasoline	99.69%	1.994E-06
High Ethanol Blends (E85)	99.69%	1.994E-06
Pre-2007 MY Diesel	94.87%	1.897E-06
2007 and later MY Diesel	88.15%	1.763E-06
CNG	100%	2.000E-06

The SO_2 conversion factors for gasoline are based on the VMT-weighted values from the Kansas City study. The updated SO_2 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.

As for other pollutants, we model E85 fueled-vehicles using the same emission rates and adjustment equations as gasoline vehicles. We set the SO_2 EF derived for gasoline vehicles to E85 vehicles. This can result in higher estimates of SO_2 from E85 vehicles, because the energy density of E85 in MOVES is estimated to be 30% lower than E10 gasoline. Thus, even though MOVES assumes the same energy consumption for E85 and gasoline vehicles, E85 vehicles are estimated to consume 43% more grams of fuel per mile.

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 SO_2 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

[j] The sulfateEmissionRate table stored sulfate and sulfur dioxide emission factors in MOVES2010. In MOVES2014 and later, it only contains sulfur dioxide emission factors.

estimated SO_2 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). MOVES3, thus, assumes a larger percentage of fuel sulfur forms sulfate emissions in conventional diesel engines. The 2007 and later MY diesel SO_2 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 SO_2 conversion factor for 2007 and later diesel (88.15%) in MOVES3 is considerably larger than the SO_2 assumed in MOVES2010b (54.16%). The reason for the large shift is the large contribution of lubricating oil to sulfate emissions accounted for in MOVES3. 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 SO_2 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 SO_2 emissions. This assumption is also consistent with our assumption for the formation of sulfate emissions from CNG engines. Lanni et al.[75] measured SO_2 and SO_4 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 SO_2 emissions we estimated a CNG sulfur content of 7.6 ppm. Ayala et al. [76] reported that the maximum allowable fuel sulfur content for use in CNG motor vehicles is 16 ppm. The Energy Information Administration reports that the fuel sulfur content of natural gas at the burner tip is less than 5 ppm.[77] In MOVES, the default sulfur level of 7.6 ppm is assumped for CNG, to be consistent with the sulfur dioxide measurements conducted by Lanni et al.[75]

9.8 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 sulfur levels to be at or below 10 ppm. When modeling these lower fuel sulfur levels, MOVES reduces the reference sulfate emission rates by ~ 10 mg/mile for pre-2007 heavy-duty diesel trucks, and ~ 1 mg/mile for light-duty gasoline vehicles.

While the sulfate calculator is important in adjusting 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 sulfate 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 SO_2 calculator, such that the SO_2 and sulfate emissions approximately achieve a mass balance with the sulfur consumed in the fuel.

Additionally, work is needed to quantity the sulfate emissions from advanced engines and emission control technologies in MOVES, including from 2010 DPF/selective-reduction-catalyst equipped diesel engines including during diesel particulate filter regeneration (see sulfate discussion in the MOVES3 Speciation report[59]), and from light-duty diesel engines, lean-burn gasoline, and direct injection gasoline vehicles. These values can be updated as 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:

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

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

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:

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

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

$$SO4_x = NonECPM \times \left(S_B \times (1 - F_B) + S_B \times F_B \times \left(\frac{x}{x_B}\right)\right)$$

$$= \boldsymbol{NonECPM \times \left(S_B \times \left[1 - F_B + F_B \times \left(\frac{x}{x_B}\right)\right]\right)}$$

$$= \boldsymbol{NonECPM \times \left(S_B \times \left[1 + F_B \times \left(\frac{x}{x_B} - 1\right)\right]\right)} \quad \textbf{Equation A-3}$$

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:

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

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 (2008[78]) and Fulper et al. (2010[79]).

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[k]. 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.

[k] The fuel sulfur content from 87 vehicles is reported in Tables 4-11 and 4-15 from the KC PM Characterization Report[78]. 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:

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

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).[69]

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).

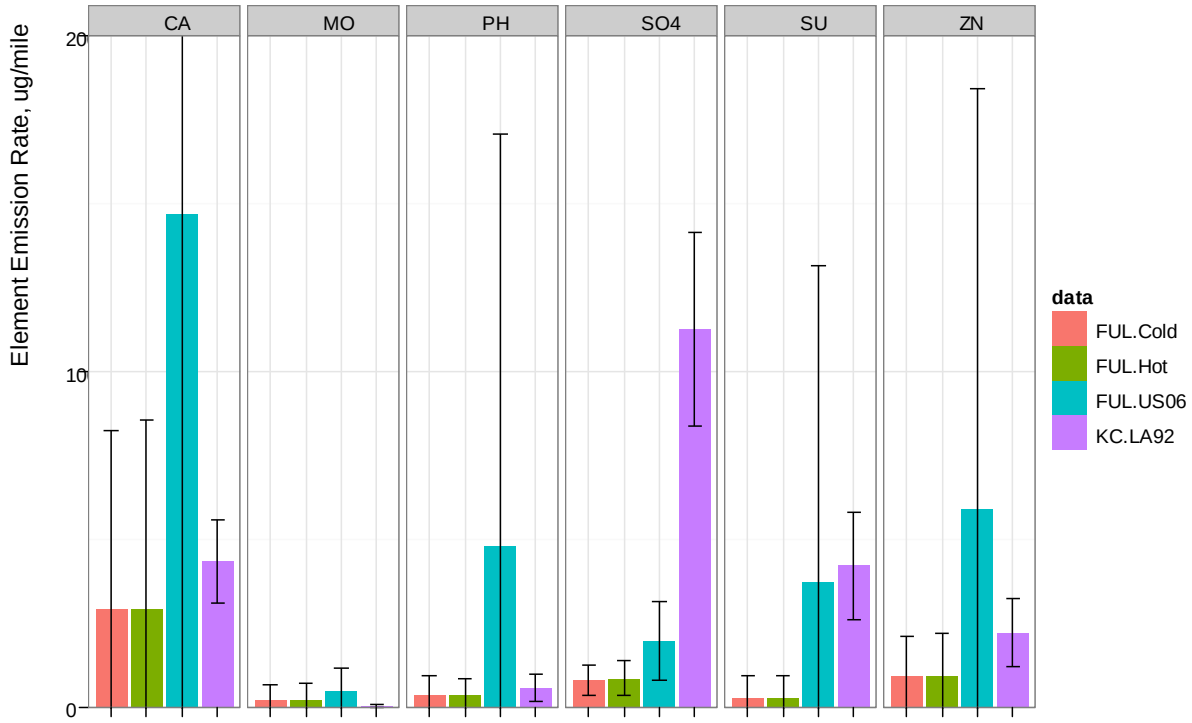


Figure A-1 contains the oil-derived metals (calcium, molybdenum, phosphorous, zinc), sulfate and sulfur emission rates from the Full Useful Life Program, from the newest vehicles from the Kansas City study (1996-2004) that are tested in the summer round. Calcium is the dominant element emitted in the 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*Cold UDDS + 0.57* 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 MOVES, 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.

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

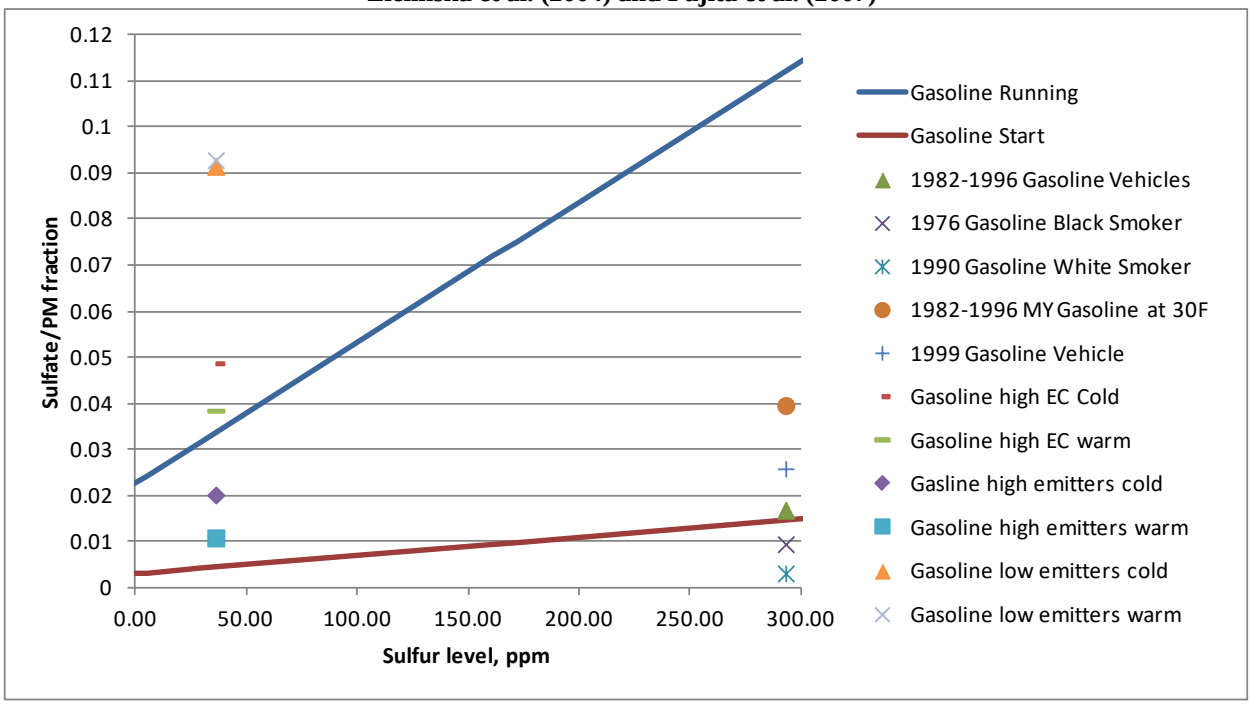
An adjustment value of 1.726 was estimated to fit the VMT-weighted average, meaning that the sulfur in the fuel and oil is 1.7 times as likely to form sulfate emissions using the fleet-average KCVES data set compared to only the summer 1996-2004 vehicles. The increase could be due to increase in oil 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 MOVES, the fuel sulfate contribution (68.7%) scales linearly with changes in fuel sulfur level, but the MOVES 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 MOVES 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. (2004[80]). 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 Zielinksa et al. (2004[80]) had a sulfur value of 293 ppm (obtained from the MOVES3 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. (2007[81]) 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. (2007[81]). 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. (2007[82]) 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. (2009[83]) 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.[84]

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 MOVES 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 DECSE[72], 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 SO_4 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 DESCE Phase 1 Study[72]

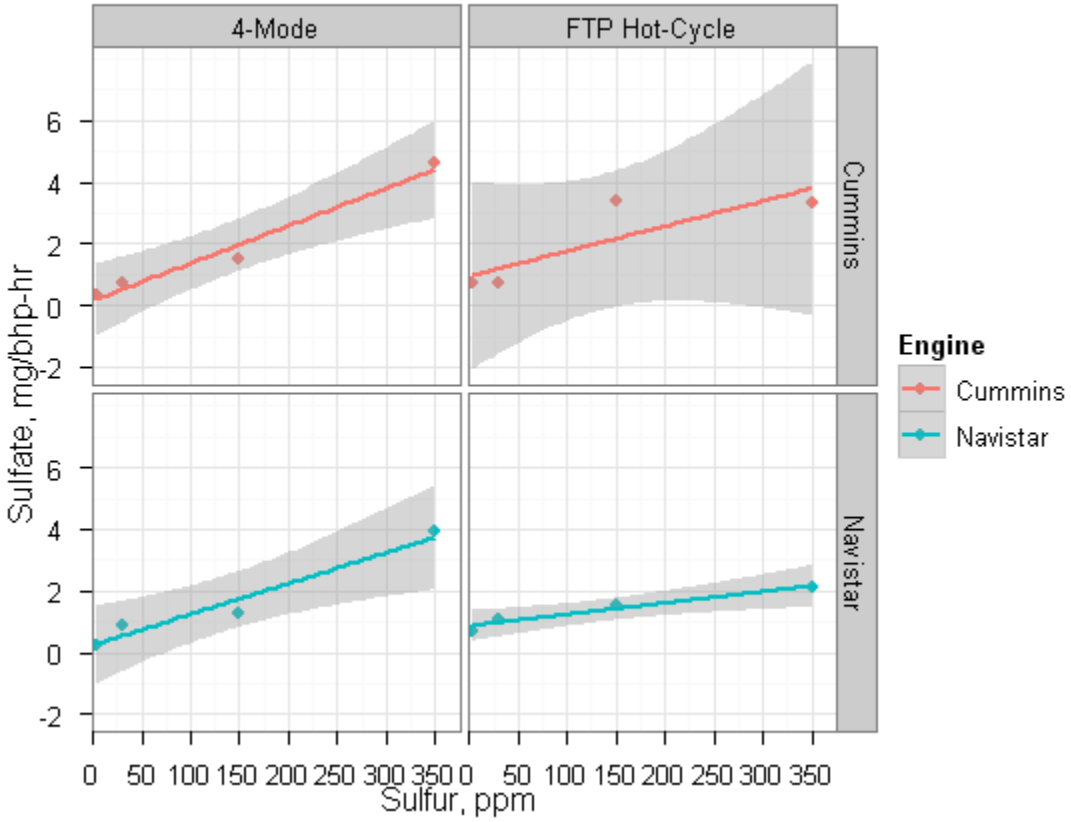
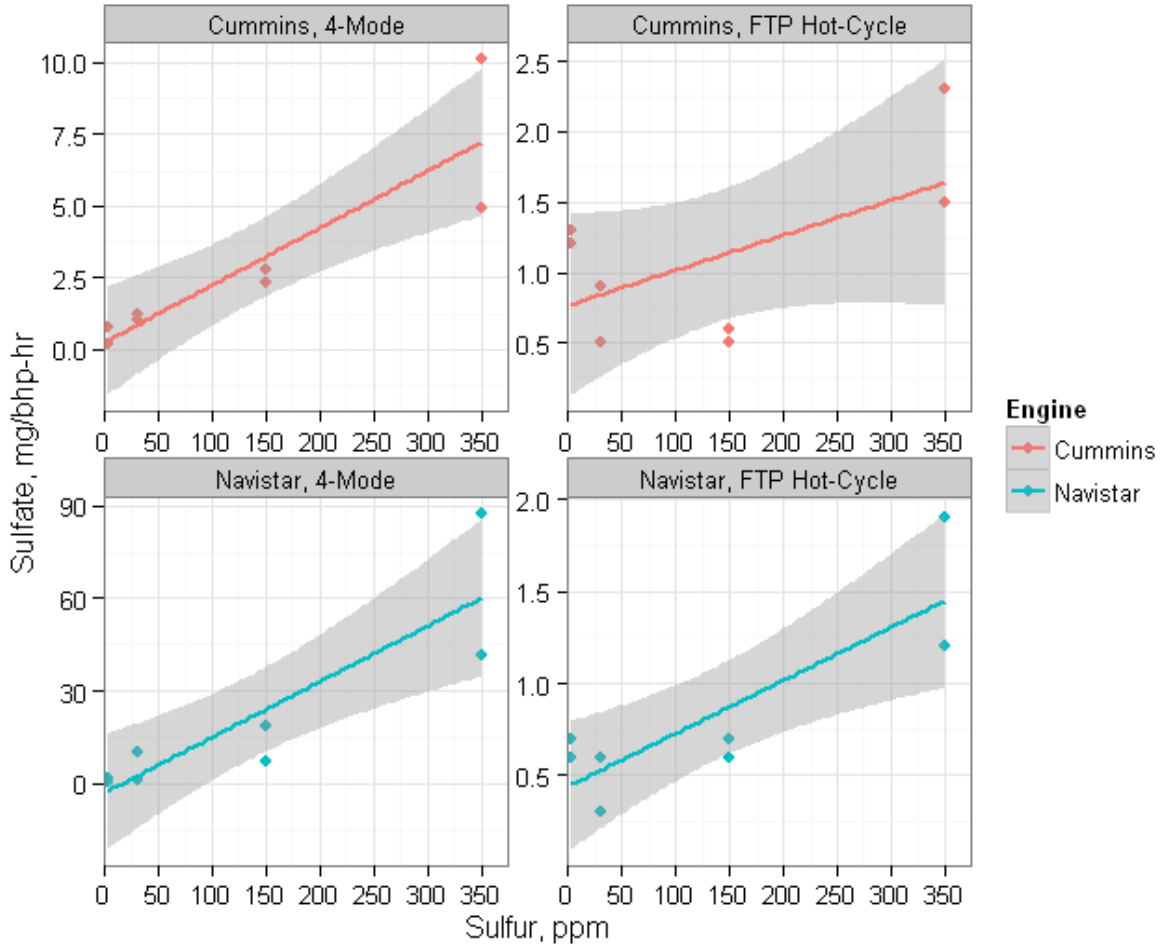


Figure A-4. Post-catalyst sulfate emissions at four fuel sulfur levels (3, 30, 150, 350) measured on a 4-mode and FTP engine test cycle, from a heavy-duty engine (Cummins) and a medium-duty engine (Navistar) from the DESCE Phase 1 Study.[72]



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.

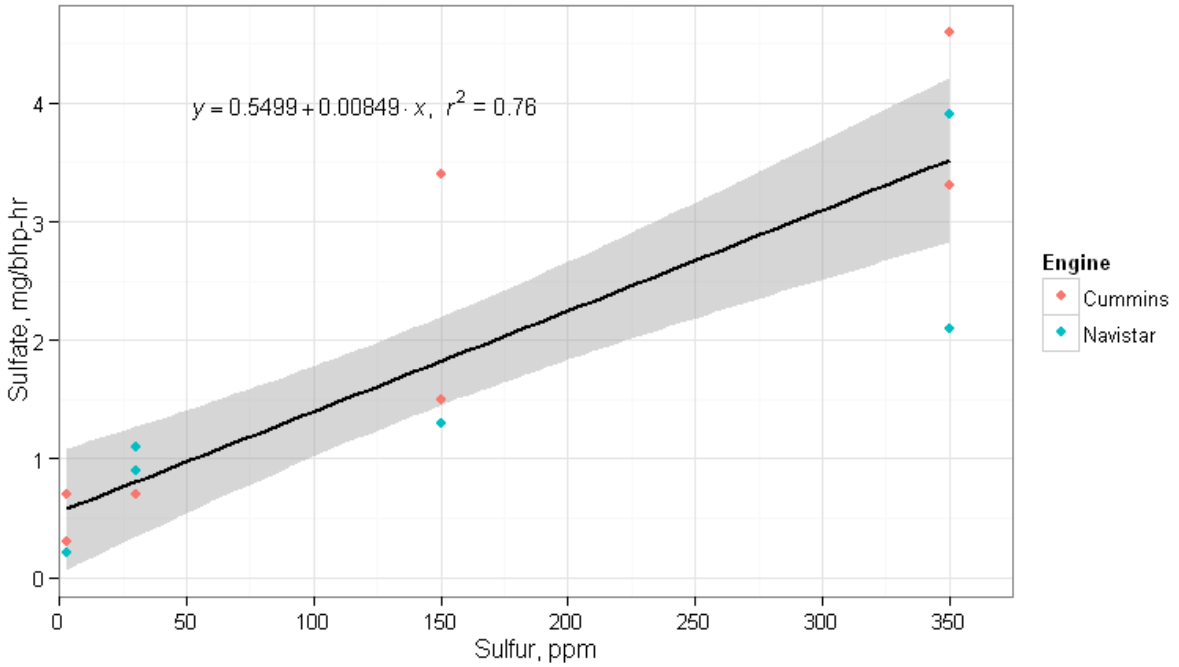


Table A-3. Estimated linear regression parameters of the engine-out sulfate emissions and fuel sulfur level data for the data displayed in Figure A-5.

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.[65] 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.

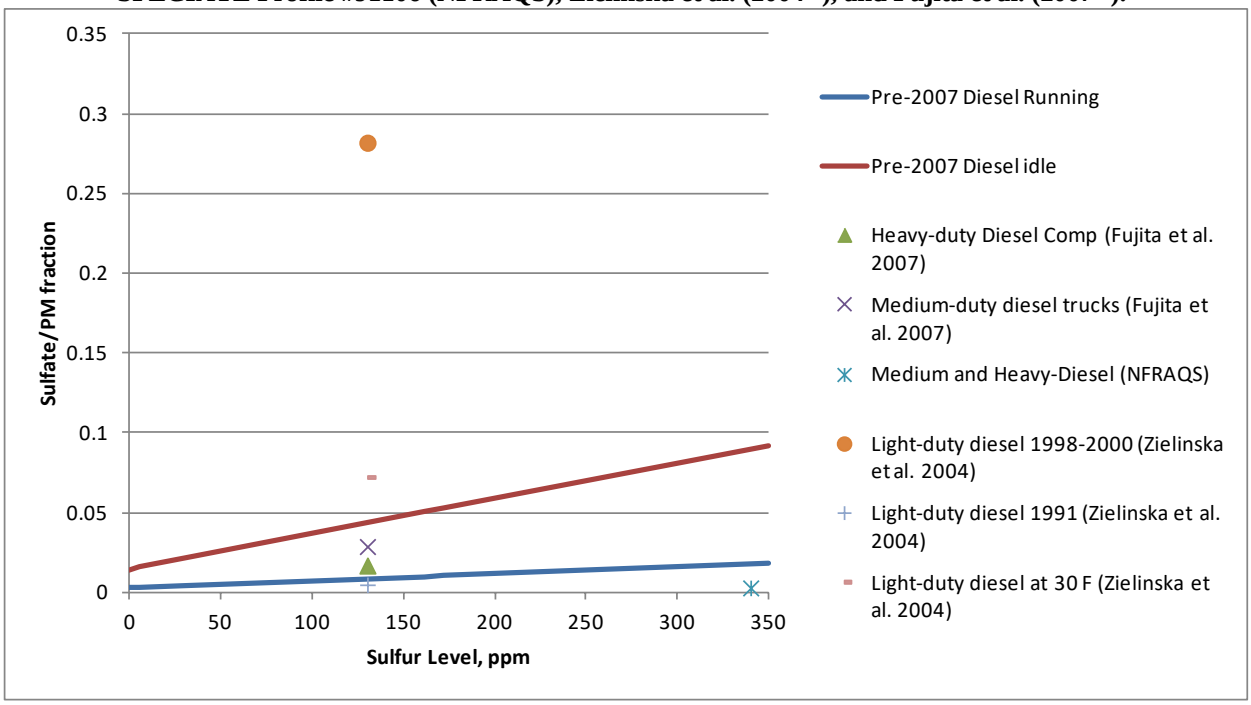
Table A-4. Estimated oil and fuel sulfate contributions to the model.

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. (2004[80]), and from heavy and medium-duty diesel trucks tested as part of the DOE Gasoline/Diesel PM Split Study reported by Fujita et al. (2007[81]). 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 timeframe, 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.[85] 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 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. (2004[80]), and Fujita et al. (2007[81]).



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. (2008[63])

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 MOVES3. 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 Estimation of Weight % Oxygenates for the Complex and Predictive Models

The complex model for carbon monoxide (Section 4.1), benzene, and 1,3-butadiene (documented in the air toxics report[1]) and has a term for wt% of oxygenate. The oxygenate wt% is calculated from the volume percent using Equation B-1.

$$Oxygenate\ (wt\%)_i = Oxygenate\ (volume\%)_i \times volToWtPercentOxy_i \qquad \text{Equation B-1}$$

Where:

Oxygenate (volume%) = is the volume percent of a fuel oxygenate. Oxygenate fuel volumes are mainly reported as % volume. For example, E10 fuel refers to a gasoline-ethanol blend fuel with approximately 10% ethanol by volume.

volToWtPercentOxy$_i$ = term used to convert from the oxygenate percentage by volume (vol%) to the mass percentage of oxygen in the fuel(mass%). volToWtPercentOxy is calculated using Equation B-2 and the values provided in Table B-1.

$$volToWtPercentOxy_i = Mass\ Fraction\ of\ Oxygen_i \times \frac{\rho_i}{\rho_F} \qquad \text{Equation B-2}$$

Where:

ρ_i = the density of the oxygenate (g/cm^3)

ρ_F = the density of the gasoline fuel, assume to be 0.75 g/cm^3

The mass fraction of oxygen, densities of the oxygenates, and calculated volToWtPercentOxy values are shown in Table B-1.

Table B-1. Volume to Weight Percent Oxygen for Gasoline Oxygenates

Oxygenate Name	Mass Fraction of Oxygen	Density of the Oxygenate (g/cm^3)	Volume to Weight Percent Oxygen (volToWtPercentOxy), assuming gasoline fuel density of 0.75 g/cm^3
Ethanol	0.3473	0.789	0.3653
MTBE	0.1815	0.7404	0.1792
ETBE	0.1566	0.7364	0.1537
TAME	0.1566	0.791	0.1651

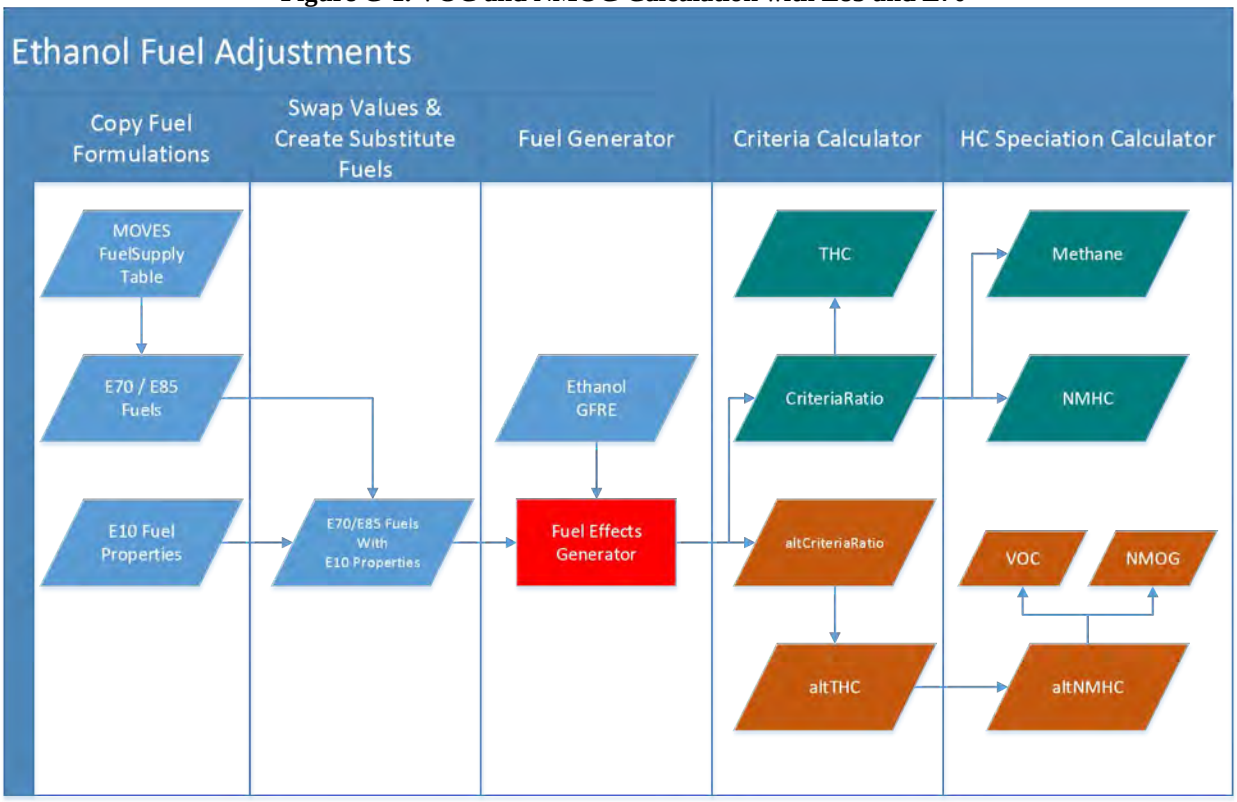
Table B-1 above contains values for Ethanol, MTBE, ETBE, and TAME. In MOVES3, we have removed MTBE, ETBE, and TAME from the fuel formulation table, and MOVES3 assumes all input fuels have zero volume of MTBE, ETBE, and TAME. However, for the complex model fuel adjustments, MOVES3 assumes the base fuel does contain volumes of these fuels, as documented in the Air Toxics Report.[1]

Appendix C High Ethanol (E85) Fuel Adjustments and HC species VOC and NMOG

As explained in Speciation of Total Organic Gas and Particulate Matter Emissions from Onroad Vehicles in MOVES3,[59] VOC and NMOG in MOVES are calculated from non-methane hydrocarbons (NMHC), which, in turn, are calculated from total hydrocarbons (THC). EPA analysis of emissions using high ethanol gasoline blends (E85 and similar) found that NMHC emissions from vehicles using these fuels were statistically significantly different from vehicles using E10 due to statistically significant differences in methane (CH_4) emissions. However, no such differences were seen for VOC or NMOG emissions (Section 7.2). Thus, MOVES has special algorithms to calculate start and running VOC and NMOG for vehicles using E85 and E70 fuels.

As depicted in Figure C-1, this algorithm requires developing a set of substitute fuel formulations that have the fuel properties needed to calculate the actual emission effects. The detailed steps of this process are described below.

Figure C-1. VOC and NMOG Calculation with E85 and E70



C.1 Copy fuel formulations

First, the high ethanol fuel formulations in the fuelFormulation table are duplicated. New fuel formulation entries are added with identical properties and new fuelFormulationID values. The new formulations will be the only formulations used in subsequent steps. The original formulations are preserved in case future MOVES algorithms require the data.

The fuelSupply table is searched for all high ethanol fuel formulations (fuel subtypes 51 and 52) and their region, fuel year, and month group noted. The matching formulations are duplicated and fuelSupply entries changed to use the new formulations. A new fuel formulation entry is created for each unique combination of fuel formulation, region, fuel year, and month group. This is done to guarantee formulation independence required by the next step.

C.2 Swap values to create substitute fuels

The E10FuelProperties table provides E10 properties by region, fuel year, and month group. Each new formulation and its associated region, fuel year, and month group is matched with an entry in the E10FuelProperties table and the new formulation's properties updated. The E10FuelProperties table contains several NULL values to use E85-specific fuel properties in estimating emissions – they are ETOHVolume, sulfurLevel, and benzeneContent and for these fuel properties, the values in the new formulation is left unaltered.

In addition, the new fuelFormulation's RVP is not altered, remaining at the high ethanol RVP for calculation of THC. In parallel, a field named "altRVP" is added to the new fuelFormulation table and the formulation's altRVP is set to the E10 fuel's RVP. The E10 altRVP will be used to estimate intermediate "altTHC" that is not reported to the user but is needed for subsequent calculations in Step 5.

C.3 Step 3 Fuel Generator

The FuelEffectsGenerator populates the CriteriaRatio table that is used to calculate THC. For ethanol fuels (fuel type 5), the data comes from equations in the GeneralFuelRatioExpression ("GFRE") table. In addition to normal THC CriteriaRatio entries, entries for THC equivalent to E10 fuel must be calculated for high ethanol fuel formulations.

Within FuelEffectsGenerator, this is accomplished by duplicating and altering the GFRE entries for fueltypeid = 5. The GFRE table is read into memory as a collection of Java objects. These objects are searched for entries that are applicable for fueltypes, THC pollutant, Running Exhaust (1) or Start Exhaust (2), and model years 2001 and later. Matching entries are duplicated. The duplicates are altered to apply to pollutant "altTHC" (10001), restricted to only fuel subtypes 51 and 52, and to begin no earlier than the 2001 model year. Further, the equations in the duplicates are altered to use "altRVP" instead of "RVP", thus making the equations generate altTHC based upon E10 RVP not E70/E85 RVP.

The GFRE objects are then processed as normal, populating the CriteriaRatio table. In addition, altTHC entries are used to populate the altCriteriaRatio table. This table has the same schema as CriteriaRatio and is used to ratio altTHC to THC in the next step.

C.4 Step 4 Criteria Calculator

Within BaseRateCalculator.sql, THC, but not altTHC, calculations proceed normally based upon data within the CriteriaRatio table. After all emission rates and adjustments to THC have been performed, altTHC is calculated using the ratio between altCriteriaRatio and CriteriaRatio:
altTHC = THC * (altCriteriaRatio.ratio for altTHC) / (CriteriaRatio.ratio for THC)

At this point, altTHC inventory or rates exist for the new high ethanol fuel formulations, running and start exhausts, and model years 2001 and later. Further, these altTHC values were derived using E10 RVP.

C.5 Step 5 HC Speciation Calculator

Within HCSpeciationCalculator.sql, methane (5) and NMHC (79) are calculated from THC for all fuel types, as normal, using speciation factors that match the fuel type. That is, for E85 emissions, methane and NMHC are calculated using the E85 methane/THC ratios.

Pollutant altNMHC (10079) is calculated from altTHC (10001) for high ethanol fuels using methane ratios for E10 fuels. AltNMHC is needed for the calculation of VOC and NMOG for high ethanol fuels. It is never reported to the user.

Pollutants VOC (87) and NMOG (80) are created from altNMHC for high ethanol fuels, running and start exhausts, and model years 2001 and later, using HC speciation factors and ethanol level for E10 fuels. VOC and NMOG are the only pollutants from E85 that are assumed to be the same as those from E10 fuels.

C.6 Step 6 Toxics and other pollutants

The calculation of toxics from E85 that are chained to VOC proceed normally, using the adjustments specific for the high ethanol fuels.

All other pollutants, including CO, NO_x, Total Energy, and PM, use the new “alt” fuel formulations that contain the input for high ethanol’s RVP, sulfur, and benzene, combined with E10 values for the remaining fuel properties.

10 References

[1] USEPA (2020). *Air Toxic Emissions from Onroad Vehicles in MOVES3*. EPA-420-R-20-022. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.

[2] USEPA (2020). *Evaporative Emissions from Onroad Vehicles in MOVES3*. EPA-420-R-20-012. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.

[3] USEPA (2020). *Fuel Supply Defaults: Regional Fuels and the Fuel Wizard in MOVES3*. EPA-420-R-20-017. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.

[4] 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.

[5] USEPA Office of Transportation and Air Quality. *Regulatory Announcement: EPA Sets Tier 3 Tailpipe and Evaporative Emission and Vehicle Fuel Standards*. EPA-420-F-008. Office of Air and Radiation. March, 2014. http://www3.epa.gov/otaq/documents/tier3/420f14008.pdf

[6] 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

[7] USEPA (2020). *Fuel Effects on Exhaust Emissions from Onroad Vehicles in MOVES3 - Draft Report*. Draft report and peer-review documents. Record ID 347138. EPA Science Inventory. July 2020. https://cfpub.epa.gov/si/si_public_record_report.cfm?dirEntryId=347138.

[8] USEPA (2020). *Exhaust Emission Rates for Light-Duty Onroad Vehicles in MOVES3*. EPA-420-R-20-019. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.

[9] Heck, R.; Farrauto, R.J. *Catalytic Air Pollution Control: Commercial Technology*. 3rd Edition. John Wiley & Sons, Hoboken, NJ, 2009.

[10] Eastwood, P. *Critical Topics in Exhaust Gas Aftertreatment (Engineering Design)*. Research Studies Press Ltd. Hertfordshire, England. 2000.

[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.

[14] Rutherford, J. A., *et al*. *Effects of Gasoline Properties on Emissions of Current and Future Vehicles–T_{50}, T_{90}, and Sulfur Effects.* Auto/Oil Air Quality Improvement Research Program. SAE Paper No. 952510. 1995.

[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.

[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).
[26] 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.
[27] Systems Research and Application Corporation. *Peer Review of the Effects of Fuel Sulfur Level on Emissions from the In-Use Tier 2 Vehicles*. Docket EPA-HQ-OAR-2011-0135, Item 1847. Charlottesville, VA. February, 2012. (available at www.regulations.gov, EPA-HQ-OAR-2011-0135-1847).
[28] USEPA Office of Transportation and Air Quality. *EPA Response to Comments on the peer review of "The Effects of Fuel Sulfur Level on Emissions from the In-Use Tier-2 Vehicles" (Fuel Sulfur Effects Report)*. Memorandum to Docket EPA-HQ-OAR-2011-0135, Item 1848. USEPA Assessment and Standards Division, Ann Arbor, MI. April 11, 2013. (available at www.regulations.gov, EPA-HQ-OAR-2011-0135-1848).
[29] Cohen, J., & Cohen, P. *Applied Multiple Regression/Correlation Analysis for the Behavioral Sciences.* 2nd Ed. Lawrence Erlbaum, Hillsdale, NJ. 1983.
[30] Engels, J.M.; Diehr, P. 2003. Imputation of missing longitudinal data: a comparison of methods. *Journal of Clinical Epidemiology*, 56:968–976.
[31] Downey R.G.; King C.V. 1998. Missing data in Likert ratings: a comparison of replacement methods. *J Gen. Psychol.* 125:175–191.
[32] Stephens, R.D. 1994. Remote sensing data and a potential model of vehicle exhaust emissions. *J Air Waste Man Assoc*. 44:1284-1292.
[33] Holmen, B.A.; Niemeier, D.A. 1998. Characterizing the effects of driver variability on real-world vehicle emissions. *Transportation Research Part D: Transport and Environment.* 3(2):117-128.
[34] Beydoun, M., & Guldmann, J. 2006. Vehicle characteristics and emissions: Logit and regression analyses of I/M data from Massachusetts, Maryland, and Illinois. *Transportation Research Part D: Transport and Environment*, 11(1), 59-76.
[35] Diggle P.J. 1988. An approach to the analysis of repeated measures. *Biometrics.* 44:959-971.
[36] Wolfinger, R.D. 1993. Covariance structure selection in general mixed models. *Communications in Statistics, Simulation and Computation.* 22(4):1079-1106.
[37] USEPA Office of Transportation and Air Quality. *Analysis of Particulate Matter Emissions from Light-Duty Gasoline Vehicles in Kansas City*. EPA-420-R-08-010. Assessment and Standards Division, Ann Arbor, MI. April, 2008. (Chapter 8).
[38] USEPA Office of Mobile Sources. *Final Regulatory Impact Assessment for Reformulated Gasoline*. EPA-420-R-93-017. Ann Arbor, MI. December, 1993.
[39] USEPA Office of Transportation and Air Quality. *Technical Support Document: Analysis of California's Request for Waiver of the Reformulated Gasoline Oxygen Content Requirement for California Covered Areas*. EPA420-R-01-016 (Docket A-2000-10, Document No. II-B-2). Transportation and Regional Programs Division, Ann Arbor, MI. June 2001.
[40] USEPA Office of Transportation and Air Quality. MOVES2010 Fuel Adjustment and Air Toxic Emission Calculation Algorithm – Development and Results. EPA-420-R-11-009. Assessment and Standards Division, Ann Arbor, MI. July, 2011. http://www.epa.gov/otaq/models/moves/documents/420r11009.pdf
[41] USEPA Office of Transportation and Air Quality. EPAct/V2/E-89: *Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles certified to Tier-2 Standards: Final Report on Program Design and Data Collection*. EPA-420-R-13-004. Assessment and Standards Division, , Ann Arbor, MI; National Renewable Energy Laboratory, Golden, CO; Coordinating Research Council, Alpharetta, GA. April, 2013.

[42] USEPA Office of Transportation and Air Quality. *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. Assessment and Standards Division, Ann Arbor, MI. April, 2013.
[43] Snedecor, George W.; Cochran, William G. *Statistical Methods*. Iowa State University Press, Ames, Iowa. 1967. (page 35.).
[44] Neter, J.: Kutner, M.H.; Nachtsheim, C.J.; Wasserman, W. Applied Linear Statistical Models. Fourth Ed., Irwin, Chicago. 1996. (Section 7.5).
[45] West, Brady T.; Welch, Kathleen B.; Galecki, Andrzej T. *Linear Mixed Models: A Practical Guide Using Statistical Software*. Taylor and Francis CRC Press. 376 pp. 2007.
[46] SAS Institute Inc. *SAS/STAT User's Guide, Version 6*. Fourth Ed., Vol. 2. Chapter 25, The LIFEREG Procedure. Pp. 997-1026. Cary, NC. 1990.
[47] Schabenberger, O. *Mixed Model Influence Diagnostics*. Paper 189-29 In: SAS Institute, Inc. Proceedings, Twenty-Ninth Annual SAS Users Group International Conference (SUGI 29), Montreal, Canada May 9-12, 2004.
[48] Energy Policy Act of 2005. Public Law 109−58, 2005; http:// www.gpo.gov/fdsys/pkg/BILLS-109hr6enr/pdf/BILLS-109hr6enr.pdf.
[49] U.S. Environmental Protection Agency. Fuels and Fuel Additives, Renewable Fuel Standard; http://www.epa.gov/otaq/fuels/renewablefuels.
[50] Energy Independence and Security Act of 2007. Public Law 110−140, 2007; http://www.gpo.gov/fdsys/pkg/BILLS-110hr6enr/pdf/ BILLS-110hr6enr.pdf.
[51] Kelly, K., Eudy, L., and Coburn, T. *Light-Duty Alternative Fuel Vehicles: Federal Test Procedure Emissions Results*. Technical Report. National Renewable Energy Laboratory, NREL/TP-540-25818, September, 1999.
[52] Karavalakis, G., Durbin, T., Shrivastava, M., Zheng, Z., Villela, M., and Jung, H. Impacts of ethanol fuel level on emissions of regulated and unregulated pollutants from a fleet of gasoline light-duty vehicles. *Fuel*. 93:549-558. March, 2012.
[53] Haibo Zhai , H. Christopher Frey , Nagui M. Rouphail , Gonçalo A. Gonçalves & Tiago L. Farias (2009) Comparison of Flexible Fuel Vehicle and Life-Cycle Fuel Consumption and Emissions of Selected Pollutants and Greenhouse Gases for Ethanol 85 Versus Gasoline, *Journal of the Air & Waste Management Association*, 59:8, 912-924.
[54] USEPA (2020). *Population and Activity of Onroad Vehicles in MOVES3*. EPA-420-R-20-023. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.
[55] USEPA (2013). *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. Assessment and Standards Division, Office of Transportation and Air Quality, Ann Arbor, MI. April, 2013.
[56] Yanowitz, J., Knoll, K., Kemper, J., Luecke, J., and McCormick R. Impact of Adaptation on Flex-Fuel Vehicle Emissions When Fueled with E40. *Environmental Science & Technology*. 2013, 47(6), 2990-2997.
[57] Haskew, H.M., and Liberty, T.F. *Exhaust and Evaporative Emissions Testing of Flexible-Fuel Vehicles. Final Report.* Coordinating Research Council. CRC Report No. E-80, August, 2011. Available at www.crcao.org.
[58] Long, T., Herrington, J., Hays, M., Baldauf, R., and Snow, R. *Air Toxic Emission from Passenger Cars Operating on Ethanol Blend Gasoline*. 104th Air and Waste Management Association Annual Conference and Exhibition, 2011, #118, 3053-3058.
[59] USEPA (2020). *Speciation of Total Organic Gas and Particulate Matter Emissions from Onroad Vehicles in MOVES3*. EPA-420-R-20-021. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.
[60] USEPA Office of Transportation and Air Quality. *Regulatory Impact Analysis: Renewable Fuel Standard Program (RFS2)*. EPA-420-R-10-006. Assessment and Standards Division, Ann Arbor, MI. February, 2010. (Appendix A).
[61] McCormick, R.; Williams, A. *Impact of Biodiesel on Modern Diesel Engine Emissions*. Project ID: FT011. National Renewable Energy Laboratory, Golden, CO. May 9, 2011. http://energy.gov/eere/vehicles/downloads/impact-biodiesel-modern-diesel-engine-emissions.
[62] Durbin, T., J. Miller, K. Johnson, M. Hajbabaei, N. Kado, R. Kobayashi, C. Vogel, F. Matsumura and P. Wong (2011). *Final Report for the CE-CERT Engine Testing Portion for the CARB Assessment of the Emissions from the*

Use of Biodiesel as a Motor Vehicle Fuel in California Biodiesel Characterization and NOx Mitigation Study. Final Report Prepared for CARB. http://www.arb.ca.gov/fuels/diesel/altdiesel/20111013_CARB%20Final%20Biodiesel%20Report.pdf.

[63] Kittelson, D. B., W. F. Watts, J. P. Johnson, C. Thorne, C. Higham, M. Payne, S. Goodier, C. Warrens, H. Preston, U. Zink, D. Pickles, C. Goersmann, M. V. Twigg, A. P. Walker and R. Boddy (2008). Effect of Fuel and Lube Oil Sulfur on the Performance of a Diesel Exhaust Gas Continuously Regenerating Trap. *Environ Sci Technol,* 42 (24), 9276-9282. DOI: 10.1021/es703270j.

[64] Khalek, I. A., T. L. Bougher, P. M. Merritt and B. Zielinska (2011). Regulated and Unregulated Emissions from Highway Heavy-Duty Diesel Engines Complying with U.S. Environmental Protection Agency 2007 Emissions Standards. *Journal of the Air & Waste Management Association,* 61 (4), 427-442. DOI: 10.3155/1047-3289.61.4.427.

[65] Allansson, R.; Maloney, C.A.; Walker, A.P.; Warren, J.P. *Sulphate Production Over the CRT: What Fuel Sulphur Level is Required to Enable the EU 4 and the EU 5 PM Standards to be Met?*. SAE Technical Paper Series. 2000-01-1875. SAE International, Warren, PA.

[66] Wall, J.; Shimpi, S.; Yu, M. *Fuel Sulfur Reduction for Control of Diesel Particulate Emissions*. SAE Technical Paper 872139. 1987. SAE International, Warren, PA.

[67] Baranescu, R. *Influence of Fuel Sulfur on Diesel Particulate Emissions*. SAE Technical Paper 881174. 1988.

[68] Hochhauser, A.; Schleyer, C.; Yeh, L.; Rickeard, D. *Impact of Fuel Sulfur on Gasoline and Diesel Vehicle Emissions*. SAE Technical Paper 2006-01-3370. 2006.

[69] Sobotowski, R.; *Test Program to establish LDV Full Useful Life PM Performance*. Memorandum to Docket EPA-HQ-OAR-2011-0135, Item 0428. USEPA Office of Transportation and Air Quality, Assessment and Standards Division, Ann Arbor, MI. March 1, 2013. (www.regulations.gov, EPA-HQ-OAR-2011-0135-0428).

[70] Clark, N.N.; Gautam, M. *Heavy-Duty Vehicle Chassis Dynamometer Testing for Emissions Inventory, Air Quality Modeling, Source Apportionment and Air Toxics Emissions Inventory*. CRC Report No. E55/59. West Virginia University Research Corporation, Morgantown, WV. August, 2007.

[71] USEPA (2020). *Exhaust Emission Rates of Heavy-Duty Onroad Vehicles in MOVES3*. EPA-420-R-20-018. Office of Transportation and Air Quality. US Environmental Protection Agency. Ann Arbor, MI. November 2020. https://www.epa.gov/moves/moves-technical-reports.

[72] US Department of Energy. *Diesel Oxidation Catalysts and Lean-NOx Catalysts. Final Report*. Diesel Emission Control – Sulfur Effects (DECSE) Program. National Renewable Energy Laboratory, Golden, CO. June 2001.

[73] Jääskeläinen, H.; Majewski, W. A. *Diesel Engine Lubricants*. www.DieselNet.com. Copyright © Ecopoint Inc. Revision 2013.01.

[74] Khalek, Imad. A.; Bougher, T. L; Merritt, P. M. *Phase 1 of the Advanced Collaborative Emissions Study*. CRC Report: ACES Phase 1. Coordinating Research Council, Alpharetta, GA. June, 2009.

[75] Lanni, T., B. Frank, S. Tang, D. Rosenblatt and D. Lowell (2003). Performance and Emissions Evaluation of Compressed Natural Gas and Clean Diesel Buses at New York City's Metropolitan Transit Authority. *Society of Automotive Engineers,*(SAE Technical Paper 2003-01-0300).

[76] Ayala, A., M. Gebel, R. Okamoto, P. Rieger, N. Kado, C. Cotter and N. Verma (2003). Oxidation Catalyst Effect on CNG Transit Bus Emissions. *Society of Automotive Engineers,*(SAE Technical Paper 2003-01-1900).

[77] Energy Information Administration. Natural Gas 1998: Issues and Trends. Chapter 2. Natural Gas and the Environment. April 1998. Available at: http://www.eia.doe.gov/oil_gas/natural_gas/analysis_publications/natural_gas_1998_issues_and_trends/it98.html.

[78] USEPA Office of Transportation and Air Quality. *Kansas City PM Characterization Study. Final Report*. EPA420-R-08-009. Assessment and Standards Division, Ann Arbor, MI. Revised by EPA Staff, April, 2008.

[79] Fulper, C. R., S. Kishan, R. W. Baldauf, M. Sabisch, J. Warila, E. M. Fujita, C. Scarbro, W. S. Crews, R. Snow and P. Gabele (2010). Methods of characterizing the distribution of exhaust emissions from light-duty, gasoline-powered motor vehicles in the US fleet. *Journal of the Air & Waste Management Association,* 60 (11), 1376-1387.

[80] Zielinska, B., J. Sagebiel, J. D. McDonald, K. Whitney and D. R. Lawson (2004). Emission Rates and Comparative Chemical Composition from Selected In-Use Diesel and Gasoline-Fueled Vehicles. *Journal of the Air & Waste Management Association,* 54 (9), 1138-1150. DOI: 10.1080/10473289.2004.10470973.

[81] Fujita, E. M., B. Zielinska, D. E. Campbell, W. P. Arnott, J. C. Sagebiel, L. Mazzoleni, J. C. Chow, P. A. Gabele, W. Crews, R. Snow, N. N. Clark, S. W. Wayne and D. R. Lawson (2007). Variations in Speciated Emissions from

Spark-Ignition and Compression-Ignition Motor Vehicles in California's South Coast Air Basin. *Journal of the Air & Waste Management Association,* 57 (6), 705-720. DOI: 10.3155/1047-3289.57.6.705.

[82] Robert, M. A., S. VanBergen, M. J. Kleeman and C. A. Jakober (2007). Size and Composition Distributions of Particulate Matter Emissions: Part 1—Light-Duty Gasoline Vehicles. *Journal of the Air & Waste Management Association,* 57 (12), 1414-1428. DOI: 10.3155/1047-3289.57.12.1414.

[83] Cheung, K. L., A. Polidori, L. Ntziachristos, T. Tzamkiozis, Z. Samaras, F. R. Cassee, M. Gerlofs and C. Sioutas (2009). Chemical Characteristics and Oxidative Potential of Particulate Matter Emissions from Gasoline, Diesel, and Biodiesel Cars. *Environ Sci Technol,* 43 (16), 6334-6340. DOI: 10.1021/es900819t.

[84] May, A. A., N. T. Nguyen, A. A. Presto, T. D. Gordon, E. M. Lipsky, M. Karve, A. Gutierrez, W. H. Robertson, M. Zhang, C. Brandow, O. Chang, S. Chen, P. Cicero-Fernandez, L. Dinkins, M. Fuentes, S.-M. Huang, R. Ling, J. Long, C. Maddox, J. Massetti, E. McCauley, A. Miguel, K. Na, R. Ong, Y. Pang, P. Rieger, T. Sax, T. Truong, T. Vo, S. Chattopadhyay, H. Maldonado, M. M. Maricq and A. L. Robinson (2014). Gas- and particle-phase primary emissions from in-use, on-road gasoline and diesel vehicles. *Atmospheric Environment,* 88 (0), 247-260. DOI: http://dx.doi.org/10.1016/j.atmosenv.2014.01.046.

[85] Zielinska, B.; McDonald, J.; Hayes, T.; Chow, Fujita, J.E.; Watson, J. 1998. *Northern Front Range Air Quality Study: Final Report. Volume B: Source Measurements*. Desert Research Institute, Reno NV. June, 1998.