
MOVES2010 Fuel Adjustment and Air Toxic Emission Calculation Algorithm – Development and Results

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

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1. Introduction

This document describes in detail the default fuels, fuel adjustment and air toxic calculation algorithms contained in the MOVES2010 model released in December 2009. It also describes the minor changes made for MOVES2010a, released in September 2010. The MOVES2010 algorithms were substantially redesigned from those contained in previous versions of the MOVES model. The revisions make the MOVES model more robust in terms of fuel modeling, easier to use, and removes a number of coding errors and problems.

This document discusses the impact of fuel properties on emissions, particularly the fuel adjustments applied to base emission results in MOVES. It details the fuel adjustment model methodology, and presents limited results pertaining to the following pollutants and their associated exhaust processes. These include the ‘running’, ‘start’ and ‘extended idle’ processes. It also includes evaporative processes for Benzene, MTBE and Ethanol where simple ratios are used. This document does not cover the impact of gasoline properties on the total hydrocarbon evaporative emission process algorithms such as permeation, vapor venting or leaks, which are described in the MOVES draft technical report on evaporative emissions (Development of Evaporative Emissions Calculations for the Motor Vehicle Emissions Simulator (Draft MOVES2009) EPA-420-P-09-006, August 2009, <http://www.epa.gov/otaq/models/moves/techdocs/420p09006.pdf>)

In general, the MOVES model calculates detailed “base emissions” on a base fuel, sums the emissions to develop total emissions for a given model year, source type and fuel type, and then applies a fuel adjustment to this aggregate emission quantity. The fuel adjustment is a weighted average for the fuels in a given area, as defined by their fuel properties and the market share listed in the MOVES fuel supply table. Air toxic emissions are calculated as a ratio to the emission of other pollutants (usually total hydrocarbons), and the ratio may or may not vary with fuel properties.

Different algorithms are used to calculate fuel effects for different fuel properties and for different air pollutants. Each is covered in a separate section of this report:

- Complex Model Algorithms for Gasoline Vehicle Air Toxic Fuel Effects - this covers benzene; 1, 3 butadiene, acetaldehyde and formaldehyde
- MTBE Complex Model (revised between December, 2009 and September, 2010) provides algorithms for emissions of methyl tertiary-butyl ether from gasoline fueled vehicles
- Algorithms for other toxics from gasoline vehicles in MOVES2010, covering ethanol, acrolein, and naphthalene

- Complex Model Algorithms for Carbon Monoxide
- Predictive Model for Total Hydrocarbon (THC) and Oxides of Nitrogen (NO_x) Fuel Effects
- MOBILE6.2 Fuel Sulfur Effects Model applies to start and running THC, CO and NO_x emissions.
- Combining the Complex/Predictive Models with the Fuel Sulfur Effects Model
- Bio-Diesel Criteria Pollutant Emission Effects
- Toxic Emissions for Diesel Vehicles
- Hydrocarbon Speciation Adjustments

The report ends with a description of the data sources for MOVES default fuels and with a section on results.

The algorithms used in MOVES2010 for gasoline and diesel vehicles were developed over 10 years ago. EPA is currently completing analysis of more recent data, representing more extensive testing, modern vehicles and engines, and fuels more representative of what is currently being sold. EPA is planning a more comprehensive fuels update that will include data from test programs being completed as part of the analysis mandated by the 2005 Energy Policy Act (EPACT) (<http://www.epa.gov/otaq/fuels.htm>) However, this document only covers analysis, code and data that were analyzed and implemented in the MOVES2010 and MOVES2010a version of the model. None of the EPAct study results were available for the MOVES2010a version of September, 2010, and are not discussed here.

As noted by the nomenclature of the above list, various existing fuel models were incorporated into the MOVES algorithm. These models are:

1. EPA Complex Model – This model was published in 1993 and is based on emissions from 1990 technology light duty vehicles. It estimates fuel effects on exhaust emissions of volatile organic compounds (VOC), carbon monoxide (CO), NO_x and air toxics; and evaporative emissions of HC, including benzene. Normal emitters and high emitters are treated separately. The output of the model compares emissions of a test fuel to the Base Fuel defined in the Clean Air Act Amendments of 1990. See the link below to download the Complex Model.

<http://www.epa.gov/otaq/rfg.htm>.

2. EPA Predictive Model – This model was originally created to evaluate a California request for a waiver of reformulated gasoline requirements. It is based on more recent data than that used for the Complex Model but only predicts VOC and NO_x. The model was revised when EPA evaluated the Renewable Fuel Standard (RFS). It is described in some detail in an EPA report (EPA 420 R-07-

004, “*Regulatory Impact Analysis: Renewable Fuel Standard Program*”, USEPA, OTAQ, Assessment and Standards Division, April 2007).

3. ARB Predictive Model – Last updated in 2006, this model predicts emissions of a test fuel compared to California Air Resources Board (ARB) Phase 3 gasoline. It estimates exhaust emissions of non-methane organic gases (NMOG), NO_x, and air toxics; and evaporative emissions of NMOG and benzene. The time period of the estimate is 2015, and all light duty vehicles (cars and light trucks) were considered in developing the model. No distinction is made in the model between normal and high emitters. This model was not explicitly included in the MOVES2010a version. The link for additional documentation is:
www.epa.gov/otaq/regs/fuels/rfg/r01016.pdf
4. MOBILE6/MOBILE6.2 – This model is a precursor to MOVES and predicts inventory emissions for mobile sources. Within MOBILE6 is a fuels module that estimates how emissions will change as a function of Reid Vapor Pressure (RVP), oxygenate and sulfur content. The sulfur portion of MOBILE6.2 is described in an EPA report. (EPA420-R-01-039, “*Fuel Sulfur Effects on Exhaust Emissions, Recommendations for MOBILE6*”, Venkatesh Rao, July 2001).

Both the Complex and Predictive models rely on the concept of a Base Fuel(s). These are specific fuel formulations at which the underlying vehicle tests that were used to generate the basic emission factors in MOVES were assumed “on average” to be conducted. In the MOVES model, a Base Fuel will produce a MOVES fuel correction factor of unity. The emission effects of other ‘target’ fuels are “ratioed” to the Base Fuel, and the subsequent product is the MOVES fuel correction factor for that ‘target’ fuel. The specific MOVES Base Fuels were chosen because they best represent the typical in-use fuel during the period in which the MOVES test vehicle emission data were collected. This choice was based on local fuel survey data of the Phoenix area during the 1995 through 2002 time period when the primary MOVES vehicle dataset was tested. (see Section 2.0 for a more complete discussion of the Base Fuels).

2. Complex Model Algorithms for Gasoline Vehicle Air Toxic Fuel Effects

This section details the calculations used to compute the air toxic emission rates in MOVES for selected air toxic compounds. These calculations were taken from the EPA Complex Model developed in the early 1990's. The air toxic compounds which use these algorithms are:

- Benzene
- Acetaldehyde
- Formaldehyde
- 1,3 Butadiene

The Complex Model algorithms are applied to running, start and extended idle emissions for gasoline fueled vehicles for all 1975 and later model years for these four pollutants. While MOBILE6 included algorithms for older technologies not included in the Complex Model, such as non-catalyst and oxidation catalyst vehicles, these algorithms are not in MOVES since these vehicles now comprise such a small portion of the fleet. In addition, while MOBILE6.2 relied on very limited data from heavy-duty gasoline vehicles to develop toxic to VOC ratios for that vehicle type, MOVES applies Complex Model algorithms to both light-duty and heavy-duty gasoline vehicles. The general structure of this section and all subsequent ones will be to describe and discuss the calculation algorithms in mathematical terms, show the underlying equation coefficients and present some limited results in graphical form for selected cases (*All results are shown in a Results section at the end of the document*).

MOVES2010a also models methyl tertiary butyl ether (MTBE), ethanol, acrolein and naphthalene. In MOVES2010a, acrolein is not affected by fuel properties and is modeled with a simple acrolein/VOC ratio as discussed later in this document. MTBE is modeled using algorithms developed from the same dataset as the Complex Model. Ethanol and naphthalene are modeled with simpler algorithms described later in this report.

2.1 Complex Model Mathematical Overview

Complex Model (CM) algorithms are used to compute the fuel effects for the pollutants benzene (exhaust and evaporative), 1,3-butadiene (exhaust), formaldehyde (exhaust) and acetaldehyde (exhaust). These algorithms were based on testing of a sample of Tier 0 vehicles (1990 and earlier model years) over a wide variety of gasoline fuel formulations. A complex statistical analysis using multivariate regression techniques was performed on the primary data set, and a set of statistical models were developed. These statistical models were originally programmed into the Unconsolidated Complex Model spreadsheet, and have now been programmed into the MOVES model and described in this document. The reader who is interested in the original test program

design, the data processing, and/or the details of the statistical analysis should refer to the original primary documents of the study.¹

The underlying goal of the CM algorithm is to compute an “air toxic ratio”. This is the ratio (or proportion) of the particular air toxic pollutant to the amount of VOC in the exhaust. In MOVES, this air toxic ratio is multiplied by the MOVES VOC estimate. Mathematically, this is shown in Equation 2-1.

$$\text{AT Emission (g/hr)} = \text{AT Ratio} * \text{VOC Emission (g/hr)} \quad \text{Eq 2-1}$$

“AT Emission” is the final emission estimate for the air toxic pollutant as reported by MOVES, and “AT Ratio” is the multiplicative factor calculated by the CM algorithm that reflects the fuel properties. The “VOC Emission” variable is the underlying VOC emissions calculated by MOVES.

In its native form, the CM model produces the (AT Ratio) by comparing the air toxic emission of a given “target” fuel to those produced by a “base” gasoline fuel (see Table 2.1). Mathematically, this relationship is shown in Equation 2-2.

$$\text{AT Ratio} = 1.0 + [(\text{AT}_{\text{Target}} - \text{AT}_{\text{Base}}) / \text{AT}_{\text{Base}}] \quad \text{Eq 2-2}$$

2.1.1 Base Fuel Concept

The ‘base’ fuel in MOVES2010a is a specific fuel at which the basic emission rates in MOVES remain uncorrected for fuel effects. MOVES2010a contains three ‘base’ fuels. There are shown in Table 2-1. Base Fuel A represents gasoline vehicles with model years 2001 and later, Base Fuel B represents gasoline vehicles with model years 2000 and earlier. Both Base Fuel A and B are used in the calculation of HC, CO and NOx emission fuel effects. Base Fuel C is used as the base fuel in the air toxic equations for all model years.

Base Fuels A and B were chosen because they best represent the typical in-use fuel during the period in which the MOVES test vehicle emission data were collected. The underlying test vehicle emission data is a large sample of in-use vehicles as they received their state transient IM240 or IM147 test. Since fuel properties were not measured on individual test vehicles during their emission test, it is presumed that the base (uncorrected) emissions best represent “on average” the presence of these fuels and their properties. The assumption of ‘best represent’ is based on local fuel survey data of the Phoenix area during the 1995 through 2002 time period when the primary MOVES vehicle dataset was tested.

Over the time period of the emission testing, the general in-use sulfur level varied due to EPA fuel sulfur regulations. As a result, MOVES2010a contains two base fuels

¹ U. S. EPA. 1993. Final Regulatory Impact Analysis for Reformulated Gasoline. December 13, 1993. <http://www.epa.gov/otaq/regs/fuels/rfg/> (ria.zip)

with the same fuel properties except fuel sulfur. Base Fuel A (a lower sulfur fuel) is used to model the 2001 and later model year vehicles, and Base Fuel B is used to model the 2000 and earlier model year vehicles. The properties of each fuel are shown in Table 2-1 below.

Base fuel C is the base fuel used only in the air toxic ratio calculations. It is a fuel which was prevalent in the early 1990's, and is the base fuel for the Complex model. This fuel formulation is central to the "centering values" and other coefficients and algorithms in the Complex model, and was the baseline fuel specified in the 1990 Clean Air Act Amendments for air toxic calculations.

2.1.2 Target Fuel Concept

The "target" gasoline is the gasoline which is to be evaluated for its effect on air toxic emissions. The target gasoline may vary by county, year and month. MOVES2010a contains a large set of fuel formulations and associated fuel market share fractions for each of the 3,222 United States counties, for each month and for calendar years 1990 and 1999 through 2012. These fuel data were assembled under EPA contract with EH Pechan who analyzed in-use fuel surveys from 2005 and made projections based statistics and EPA fuel regulations. In addition, to the large set of built-in fuel data, the user may enter their own fuel formulations and market share information, if available. Note, that the use of a 'base' fuel as a 'target' fuel will produce a fuel correction of unity.

Table 2-1 MOVES Base Fuel Properties			
Fuel Property Name	Base Fuel A	Base Fuel B	Base Fuel C
Fuel Sub-Type	Conventional Gas	Conventional Gas	Conventional Gas
RVP	6.9 psi	6.9 psi	8.7 psi
Sulfur Level	30.0 ppm	90.0 ppm	338.0 ppm *
ETOH Volume	0.0 %	0.0 %	0.0 %
MTBE Volume	0.0 %	0.0 %	0.0 %
ETBE Volume	0.0 %	0.0 %	0.0 %
TAME Volume	0.0 %	0.0 %	0.0 %
Aromatic Content	26.1 %	26.1 %	26.4 %
Olefin Content	5.6 %	5.6 %	11.9 %
Benzene Content	1.0 %	1.0 %	1.64 %
E200	41.1 %	41.1 %	50.0 %
E300	83.1 %	83.1 %	82.0 %
Volume to percent Oxygen	0.0 %	0.0 %	0.0 %

• Air toxic computation is not a function of sulfur level

For both the “Target” and “Base” fuels, the overall Complex model consists of ten individual, statistically derived models (see Section 2.2 below for more details). Each of these ten fuel models predicts emissions as an exponential function of fuel parameters and associated coefficients. Each has a weighting factor which varies by vehicle model year that is used to weight the contribution of all ten models into a composite result.

The MOVES algorithm to compute these emission effects is complex and is detailed in the next section. In summary, for each of the ten Complex Model sub-models, MOVES sums the coefficients for each model parameter, calculates the difference between the fuel value and an average fuel value, multiplies the coefficient sum by this difference, computes the sum of the resulting values across the complex model parameters and computes the exponential function of this value.

MOVES then calculates a ratio between the exponential values for the target and base fuels for each of the Complex Model sub-models. The sub-model ratios are weighted together to create a weighted average fractional difference in air toxic emissions between the base and target fuels. This information is used to predict the toxics emissions for each target fuel. Similar calculations are used to predict the VOC emissions for the same fuels, and the resulting ratios of the predicted toxics and VOC are calculated.

2.2 Complex Model Mathematical Algorithm

The Complex Model algorithm is presented in this section in a series of nine calculation steps. Each variable is defined in the steps and where and in some cases an example calculation is provided.

2.2.1 Step 1

This series of steps are used only for pollutants:

Benzene,
1,3-butadiene,
Formaldehyde
Acetaldehyde

They are performed for each of the MOVES emission processes:

running
start
evaporative processes

There are up to 64 different Complex Model parameter (cmpID) variables that represent the effects of individual fuel parameters and cross products of individual fuel parameters determined from statistical analysis of the data. Each of the ten Complex Model sub-models has coefficients that must be added. The addition for each parameter is done across each model.

The variable baseSumCoeff is the sum of coefficients for the base fuel, and the variable targetSumCoeff is the sum of coefficients for the target fuels. The structure of the table containing the coefficients is given in Table 2-2.

$$\text{basesumcoeff} = \text{coeff1} + \text{coeff2} \quad \text{Eq 2-3a}$$

$$\text{targetsumcoeff} = \text{coeff1} + \text{coeff2} \quad \text{Eq 2-3b}$$

The calculations are performed for each fuel-type (i.e., gasoline and E-85 only), for each fuel formulation, for each fuel model year combination and for all cmpID variables (denoted as cmpID in Table 2-2). Currently, the variable “coeff3” is not used in the calculation. It is reserved for possible future use.

Table 2-2 ComplexModelParameters		
Fields	Datatype	Description
polProcessID	smallint(6)	PK: standard polProcessID variable
fuelModelID	smallint(6)	PK: basic fuel and technology model index
cmpID	smallint(6)	PK: all fuel property variable
coeff1	float	First order coefficients used in calculations
coeff2	float	Second order coefficients used in calculations
coeff3	float	Third order coefficients (placeholder) used in calculations. None are currently used.

2.2.2a Step 2a

In this step 2a, the baseSumCoeff variable computed in Step 1 along with two additional variables “baseValue” and “centeringValue” are used to calculate a subsequent variable BaseProd. This calculation is performed only for the ‘base’ fuel (an analogous calculation is performed for the target fuel). Like Step 1 this calculation is performed for each pollutant / process / fuel-type / fuelformulation (base only) / fuelModelID and cmdID combination. Mathematically, the equation is given by Eq 2-4a.

$$\text{Baseprod} = \text{basesumcoeff} * (\text{baseValue} - \text{centeringValue}) \quad \text{Eq2-4a}$$

The variable “baseValue” is found in Table 2-1 for all of the parameters. The ‘baseValue’ variable and the “centeringValue” variable are listed. The table MeanFuelParameters has the following structure as used in MOVES.

```
fueltypeid
modeleargroupid
fuelparameterid
fuelparametername
basevalue
centeringvalue
```

The baseValue variable is the actual value for the base fuel (i.e., sulfurlevel, RVP, E200, etc). The “centering value” a mean value used in the calculations.

Some cmdIDs describe the product of two fuel parameters such as oxygen and RVP. This special case is illustrated in Eq2-4b for a baseprod for the cmpID that is the product of oxygen and RVP.

$$\text{Baseprod} = \text{basesumcoeff} * (\text{Oxygen} - \text{Oxygen centering value}) * (\text{RVP} - \text{RVP centering value}) \quad \text{Eq2-4b}$$

Table 2-3 MeanFuelParameters		
Fields	Datatype	Description
polProcessID	smallint(6)	PK: standard polProcessID variable
fuelTypeID	smallint(6)	PK: fuelTypeID = 1 only
modelYearGroupID	int(11)	PK: two new mygIDs added
fuelParameterID	Smallint(6)	PK: major fuel property variable
baseValue	float	Baseline fuel properties.
centeringValue	float	Fuel parameter mean value used in calculations.
stdDevValue	float	Fuel parameter standard deviation used only in HC and NOx calculations.

2.2.2b Step 2b

In this step 2b, the targetSumCoeff variable (calculated in Step 1) along with the variables “fuelParameter” and “centeringValue” are used to calculate a subsequent variable TargetProd. This calculation is performed for each of the target fuels which are being evaluated. Like Step 1 this calculation is performed for each pollutant / process / fuel-type / fuelformulationID (target fuels only) / fuelModelID and all possible cmdID combinations. Mathematically, the equation is given by Eq 2-5a. The variable “centeringValue” comes from the *MeanFuelParameters.xls* table. The fuelparameter variable is the particular fuel parameter for the target fuel (i.e., sulfurlevel, RVP, E200, etc) that the user wishes to evaluate. The calculation is performed separately for each fuel parameter.

$$\text{Targetprod} = \text{targetSumCoeff} * (\text{fuelparameter} - \text{centerValue}) \quad \text{Eq 2-5a}$$

In some cases for the Target fuel, a particular cmdID may include a fuel parameter which is a product of two fuel parameters. This special case is illustrated in Eq2-5b for a Targetprod that is the product of oxygen and RVP.

$$\text{Targetprod} = \frac{\text{Targetumcoeff} * (\text{Oxygen} - \text{Oxygen centering value}) * (\text{RVP} - \text{RVP centering value})}{\text{RVP} - \text{RVP centering value}} \quad \text{Eq2-5b}$$

2.2.3 Step 3

In this step the variables eBaseProdSum and eTargetProdSum are calculated for each pollutant, process, fuel-typeID, fuel-formulationID (base and target), and fuelModelID combination. The variables eBaseProdSum and eTargetProdSum are the exponential sum of each of the individual BaseProd and TargetProd variables. The sums are across all of the possible cmdID (1 to 64) groups.

$$\text{eBaseprodSum} = \text{EXP} [\text{SUM}(\text{Baseprod}) \text{ where cmdID} = 1 \text{ to } 64] \quad \text{Eq2-6a}$$

$$\text{eTargetprodSum} = \text{EXP} [\text{SUM}(\text{Targetprod}) \text{ where cmdID} = 1 \text{ to } 64] \quad \text{Eq2-6b}$$

In cases where the SUM(Baseprod) or SUM(Targetprod) equals zero, the value of eBaseprodSum or eTargetprodSum is set to zero rather than calculated as unity.

2.2.4 Step 4

In this step the variable Ratio1 is calculated for each pollutant, process, fueltypeID, fuelModelID, fuelformulationID (the unchanging base fuel and variable target fuel) and fuelModelID combination using Equation 2-7. There are eleven fuelModelID's for the primary exhaust air toxic pollutants.

$$\text{Ratio1} = \left(\frac{\text{eTargetprodSum}}{\text{eBaseprodSum}} \right) - 1.0 \quad \text{Eq2-7}$$

2.2.5 Step 5

In this step, the variable Ratio2 is computed by multiplying Ratio1 by a fuelModelWtFactor variable. This accounts for the mix of technologies and high emitters by model year. Each of the ten fuel models has an associated weighting factor which is a function of ageID, and two broad model year groups (1960-2000 and post-2000). The structure of the table is shown in Table 2-4, and the names of the individual fuel models for air toxic emissions are provided in Table 2-5. The individual fuel models represent fuel metering, EGR, catalyst and air injection technology groupings, as well as high emitters. The weighting factors account for the prevalence of each type of vehicle.

The weighting factors which are used in MOVES differ from those used in the original Complex model. They vary by model year group because of the changing importance of technology groupings (the original does not vary), and 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). The fraction of high emitters now varies with age. It ranges from 0.01 percent at age zero to 32.8 percent at 30 years.

Table 2-4 FuelModel Weighting Factors		
Fields	Datatype	Description
fuelModelID	smallint(6)	PK: basic fuel and technology model index
modelYearGroupID	int(11)	Only two groups
ageID	smallint(6)	Age 0 through 30
fuelModelWtFactor	float	Weight factor that sums to unity for each fuelModelID and modelYearGroupID

Table 2-5 FuelModel Names	
Fuel Model ID	Fuel Model Name
1	PFI & 3way & No Air & EGR
2	PFI & 3way & No Air & No EGR
3	TBI & 3way & No Air & EGR
4	PFI & 3way+Ox & Air & EGR
5	PFI & 3way & Air & EGR
6	TBI & 3way & Air & EGR
7	TBI & 3way+Ox & Air & EGR
8	TBI & 3way & No Air & No EGR
9	CARB & 3way+Ox & Air & EGR
10	All High Emitters
11	All Tier2

$$\text{Ratio2} = \text{Ratio1} * \text{fuelModelWtFactor} \quad \text{Eq2-8}$$

Note that FuelModel = 11 (the All Tier2 model) is not part of the calculation or the weighting (it currently receives a weighting factor of zero). It is reserved for future use.

2.2.6 Step 6

In this step, the Ratio2 variables are summed across the ten fuel models. This produces the variable atDifferenceFraction. It is a weighted sum of all of the fuel models and the base and target fuel effects. In essence, it is the fractional difference in air toxic emissions between the base and target fuels. It is calculated for each combination of pollutant, process, fueltypeID, ageID and fuelformulationID.

$$\text{atDifferenceFraction} = \text{SUM}(\text{Ratio2}) \text{ where } i = 1, \text{max}(\text{fuelmodels}) \quad \text{Eq2-9}$$

$$\frac{\text{fuelmodel [i]}}{\text{max}(\text{fuelmodels})} = 10 \quad \text{for air toxic pollutants}$$

2.2.7 Step 7

In this step the variable RelATEmissions is calculated for the Target fuel using Equation 2-10. This variable represents the air toxic emissions on the target fuel with no other adjustments. The variable RelATEmissions includes the air toxic emissions effect of the change in fuel properties of the Target fuel versus the Base fuel. If the base fuel were identical to the Target fuel, the variable atDifferenceFraction would be zero and the RelATEmissions would be the same as the atBaseEmissions.

The atBaseEmissions are the air toxic emission rates in units of grams per mile, and are a function of month of the year. They were taken directly from the Complex Model Spreadsheet “*CM Final.xls*”. They are the base air toxic emissions for the Base Fuel in the air toxics model. These base emissions were calculated from air toxic emission data from the Tier 0 vehicles in the original air toxic / fuel effects studies on which the Complex Model was based. They are used in conjunction with similar VOC emissions (see Step 8 below) to compute a final air toxic to VOC emission ratio which is used in the MOVES model. The MOVES air toxic algorithm is based on the assumption that within a fuel model group (i.e., technology group) the air toxic pollutant to VOC ratio has remained constant even as vehicle emission standards have been lowered from Tier0 to Tier2 levels. When the results of the EPACT test program are fully available, this assumption will be re-evaluated and new ratios / fuel models may be developed for Tier2 vehicles. The “All Tier2” fuel model is currently a placeholder for these new values / coefficients.

$$\text{RelATEmissions} = \text{atBaseEmissions} + \text{atBaseEmissions} * \text{atDifferenceFraction} \quad \text{Eq2-10}$$

2.2.8 Step 8

Steps 1 through 7 are repeated for the VOC pollutant. Only the final equation where the RelVOCEmissions variable is shown in Equation 2-11 is repeated. It is the denominator for the final air toxic to VOC ratio. This is NOT the computation of the standard VOC pollutant in MOVES. These steps compute a VOC value for the variables atDifferenceFraction and RelATEmissions. Like the air toxic pollutant, the atBaseEmission value for VOC was also based the original testing of Tier0 vehicles.

$$\text{RelVOCEmissions} = \text{VOCBaseEmissions} + \text{VOCBaseEmissions} * \text{atDifferenceFraction} \quad \text{Eq2-11}$$

2.2.9 Step 9

This step in Equation 2-12 calculates the final air toxic to VOC ratio which is used in the MOVES model. This algorithm is used for processes of running and start and for pollutantID {20, 24, 25 and 26}. It is used only for gasoline fueled vehicles. It shall be computed for each pollutant-process, fuelformulationID, and monthGroupID.

$$\text{atRatio} = \text{RelATEmissions} / \text{RelVOCEmissions} \quad \text{Eq2-12}$$

The variable atRatio is used in MOVES to compute the air toxic emissions for benzene, 1,3-butadiene, formaldehyde and acetaldehyde. This is done by multiplying the appropriate atRatio by the final MOVES VOC emission rate after fuel, temperature and I/M effects have been applied.

2.3 MTBE Complex Model Algorithm

2.3.1 MTBE Exhaust Model

As of calendar year 2008, MTBE (MOVES pollutantID = 22) has been almost completely phased-out of the fuel supply of the United States due to ground water contamination concerns. Thus, its inventory levels in the MOVES output from default inputs should be very small if not zero in future years. It is present in the MOVES model as mostly a legacy pollutant for calendar years 1990, 1999 – 2005. However, the MTBE fuel volume is a user input, and MOVES has the capability to calculate MTBE emissions for any calendar year.

The MTBE Exhaust model was developed from a simple empirical analysis of MOBILE6.2 outputs. MOBILE6.2 relied on a draft MTBE fuel effects model.^{2,3} This process included several detailed MOBILE6.2 runs, and a simple regression of the exhaust MTBE / VOC ratio versus MTBE fuel volume. A quadratic equation fixed at the origin was found to be the best fit. The equation is shown in Equation 2-13 and the parameters are shown in Table 2-6. The same equation is used for both start and running processes.

$$\text{MTBE/VOC ratio} = A * \text{MTBEVolume} + B * (\text{MTBEVolume})^2 \quad \text{Eq2-13}$$

Where

A = ComplexModelParameters.coeffA
 B = ComplexModelParameters.coeffB

**Table 2-6
 MOVES MTBE Exhaust Calculation Coefficients**

polProcessID	Process Description	Coeff A	Coeff B
2201	Running Exhaust	0.00007809	0.00007537
2202	Start Exhaust	0.00007809	0.0007809

Like the other air toxic ratios, the MTBE / VOC ratio is multiplied by the MOVES VOC emission factors to produce a MOVES MTBE emission factor in the

² Wyborny, L. 1998. Methyl Tertiary Butyl Ether (MTBE) Emissions from Passenger Cars. Draft Technical Report. U. S. Environmental Protection Agency, Office of Mobile Sources. April, 1998.

³ Rich Cook and Edward L. Glover. 2002. Technical Description of the Toxics Module for MOBILE6.2 and Guidance on Its Use for Emission Inventory Preparation. Assessment and Standards Division, Office of Transportation and Air Quality, Ann Arbor, MI. Report No. EPA420-R-02-011. <http://www.epa.gov/otaq/models/mobile6/r02029.pdf>

appropriate units (i.e., grams per hour, grams per start, grams per mile). In MOVES the MTBE / VOC ratio ranges from 0.015 to 0.15 in cases where MTBE is present in the fuel. The MTBE ratio is 0.000 in cases where no MTBE is present in the fuel.

2.3.2 MTBE Evaporative Model

MTBE ratios are estimated using algorithms originally developed for MOBILE 6.2, using the MTBE fuel effects model cited above. However, evaporative emissions processes for MOVES differ from those in MOBILE6.2. Thus, algorithms for hot soak in MOBILE6.2 are used for vapor venting and refueling vapor loss in MOVES, and algorithms for running loss are used for fuel leaks and refueling spillage loss. The MOBILE6.2 algorithm for resting loss is used for permeation.

The equation for MTBE fuel vapor venting and refueling displacement vapor loss:

$$\text{MTBE / VOC} = \text{MTBEVolume} * (24.2050 - 1.7460 * \text{RVP}) / 1000.0$$

The equation for MTBE fuel leaks and refueling spillage loss:

$$\text{MTBE / VOC} = \text{MTBEVolume} * (17.8538 - 1.6622 * \text{RVP}) / 1000.0$$

The equation for MTBE Permeation:

$$\text{MTBE / VOC} = \text{MTBEVolume} * (22.1980 - 1.7460 * \text{RVP}) / 1000.0$$

2.4 Benzene Evaporative Model Algorithm

The equations for Benzene evaporative emissions are simpler than the ones used for exhaust Benzene, and there are no Base fuels in the equations.

The equation for Benzene Permeation is:

$$\text{Benzene / VOC} = (\text{BenzeneContent} * (-0.02895 * \text{OXY} - 0.080274 * \text{RVP} + 1.3758) / 100.0) + (0.77 * (\text{benzeneContent} * (-0.02895 * \text{ETOHVolume} * 0.3488 - 0.080274 * \text{RVP} + 1.3758) / 100.0) * \text{ETOHVolume} / 10.0)$$

This equation is based on the diurnal emissions algorithm from MOBILE6.2. The diurnal emissions equation accounts for impacts of changing oxygenate, RVP and fuel benzene levels. However, a study of permeation emissions suggests that the ratio of benzene from permeation to total VOC is about 1.77 times higher than the ratio associated with evaporation.⁴ Thus the ratio predicted by the diurnal emissions algorithm was multiplied by 1.77.

⁴ Haskew, H. M., Liberty, T. F., and McClement, D. 2004. Fuel Permeation from Automotive Systems. Prepared for the Coordinating Research Council by Harold Haskew and Associates and Automotive Testing Laboratories, Inc. September 2004. CRC Project No. E-65. <http://www.crao.com>.

For other evaporative processes, equations for hot soak in MOBILE6.2 are used:

$$\text{Benzene / VOC} = (\text{BenzeneContent} * (-0.03420 * \text{OXY} - 0.080274 * \text{RVP} + 1.4448) / 100.0)$$

Where OXY is:

$$\begin{aligned} \text{OXY} = & \text{ ETOHVolume} * 0.3488 + \text{ MTBEVolume} * 0.1786 + \text{ ETBEVolume} * 0.1533 \\ & + \text{ TAMEVolume} * 0.1636 \end{aligned}$$

3. Algorithms for Ethanol, Acrolein and Naphthalene from Gasoline Vehicles in MOVES2010

3.1 Ethanol

Ethanol emissions in MOVES are calculated by applying an Ethanol / VOC ratio to the calculated VOC emissions in MOVES. Equation 3-1 is used.

$$\text{Ethanol} = \text{Ethanol/VOC Ratio} * \text{VOC} \quad \text{Eq3-1}$$

For vehicles running on 10% ethanol, 2.39 percent of exhaust VOC is estimated to be ethanol. This estimate is based on tests on 9 vehicles from 4 test programs.^{5, 6, 7, 8} MOVES also has ethanol to VOC ratios for E5 and E8, based on linear interpolation from the E10 value (0.01195 for E5 and 0.01912 for E8). The exhaust ethanol / VOC ratios for gasoline fuels (i.e. pure gasoline or E10 or less) are shown in Table 3-2.

Ethanol Fuel Volume (%)	Ethanol / VOC Ratio
0	0.00000
5	0.01195
8	0.01912
10	0.02390

Toxic to VOC ratios for E85 and E70 are given in Table 3-3. E85 exhaust ratios for all pollutants except naphthalene were obtained from data on seven vehicles from a 1995 test program in EPA's Office of Research and Development, along with data from a 2007 test program at Southwest Research Institute and a 2005 test program at Environment

⁵ Southwest Research Institute, 2007. Flex Fuel Vehicles (FFVs) VOC/PM Cold Temperature Characterization When Operating on Ethanol (E10, E70, E85). Prepared for U. S. Environmental Protection Agency.

⁶Environment Canada, 2007. Comparison of Emissions from Conventional and Flexible Fuel Vehicles Operating on Gasoline and E85 Fuels. ERM Report No. 05-039, Emissions Research Division.

⁷Durbin T. D., Miller J. W., Younglove T., Huai T., Cocker K., 2007. Effects of fuel ethanol content and volatility on regulated and unregulated exhaust emissions for the latest technology gasoline vehicles. Environmental Science and Technology 41, 4059-4064.

⁸ U. S. EPA, 1995. Office of Research and Development, unpublished data.

Canada.^{9,10,11} E70 exhaust ratios are from the 2007 test program at Southwest Research Institute cited above.⁹ E85 benzene evaporative emission ratios were derived from speciation data collected as part of the Auto/Oil test program in the early 1990's.¹² E85 benzene permeation ratios are from the CRC E-65 test program.⁴ Ratios for evaporative and permeation emissions from E70 fuel were estimated by multiplying the E85 ratios by 70/85.

Table 3-3 Ethanol / VOC Ratios for High Ethanol Fuels		
Ethanol Fuel Volume	Process	Ethanol / VOC Ratio
E85	Running	0.5348
E85	Start	0.5348
E85	Permeation	0.5940
E85	Fuel Vapor Venting	0.6123
E85	Fuel Leaks	0.6123
E85	Refueling Vapor Loss	0.6123
E85	Refueling Spillage	0.6123
E70	Running	0.7036
E70	Start	0.7036
E70	Permeation	0.4892
E70	Fuel Vapor Venting	0.5042
E70	Fuel Leaks	0.5042
E70	Refueling Vapor Loss	0.5042
E70	Refueling Spillage	0.5042

3.2 Acrolein and Naphthalene

The toxic to VOC ratio for acrolein carries over from MOBILE6.2. Acrolein is found only in exhaust. Naphthalene is carried over from the National Mobile Inventory Model (NMIM).¹³ Exhaust naphthalene and other PAH emissions are estimated as a ratio

⁹ Southwest Research Institute. 2007. Flex Fuel Vehicles (FFVs) VOC/PM Cold Temperature Characterization When Operating on Ethanol (E10, E70, E85). Prepared for U. S. Environmental Protection Agency. Available in Docket EPA-HQ-OAR-2005-0161.

¹⁰ Environment Canada. 2007. Comparison of Emissions from Conventional and Flexible Fuel Vehicles Operating on Gasoline and E85 Fuels. ERM Report No. 05-039, Emissions Research Division. Available in Docket EPA-HQ-OAR-2005-0161.

¹¹ Graham, L. A.; Belisle, S. L. and C. Baas. 2008. Emissions from light duty gasoline vehicles operating on low blend ethanol gasoline and E85. Atmos. Environ. 42: 4498-4516.

¹² Auto/Oil Air Quality Improvement Research Program. 1990. Phase 1 Working Data Set (published in electronic form). Prepared by Systems Applications International, San Rafael, CA.

¹³ Michaels, H., Brzezinski, D., Cook, R. 2005. EPA's National Mobile Inventory Model (NMIM), A Consolidated Emissions Modeling System for MOBILE6 and NONROAD. U. S. EPA, Office of

to PM in NMIM. This approach is used, even though naphthalene is found in the gas, semi-volatile and particle phase, because there is generally reasonable correlation between PAH and PM emissions. However, for future versions of MOVES, PAH exhaust emissions will be apportioned into the gas and particle phase, and gas phase PAHs such as naphthalene will be estimated using toxic/VOC ratios and particle phase PAHs will be estimated using toxic to OC2.5 (organic carbon less than 2.5 microns) ratios. Evaporative naphthalene is estimated as a ratio to VOC in MOVES2010a.

Table 3-3 Toxics Ratios for Acrolein and Naphthalene from Gasoline Vehicles			
Pollutant	Emission Type	Ratio Type	Ratio
Acrolein	Exhaust	VOC	0.00063
Naphthalene	Exhaust	PM	0.0880
Naphthalene	Evaporative and Permeation	VOC	0.0004

4. Complex Model Algorithms for Carbon Monoxide Fuel Effects

This section describes in detail the calculations used to compute the fuel effects for carbon monoxide emission in MOVES. These calculations were taken from the EPA Complex Model developed in the early 1990's. The algorithms include methodologies for calculating running and start emissions from gasoline vehicles. The general structure of this section will be to describe and discuss the calculation algorithms in mathematical terms, show the underlying equation coefficients and present some limited results in graphical form for selected cases.

The Complex Model (CM) algorithm is used to compute the fuel effects for carbon monoxide. This algorithm was developed in the mid-1990's based on testing of a sample of mostly Tier0 vehicles (1993 and earlier model years) over a wide variety of gasoline fuel compositions. A complex statistical analysis using multivariate regression techniques was performed on the primary database and a set of statistical models were developed. These statistical models were originally programmed into the Unconsolidated Complex Model spreadsheet, and have now been programmed into the MOVES model and described in this document. The reader who is interested in the original test program design, the data processing, and/or the details of the statistical analysis must refer to the original primary documents of the study.

<http://www.epa.gov/oms/models.htm>

The algorithm for the Complex Model for CO emission fuel effects is almost completely analogous to the Complex Model for air toxic emissions. However, there are some important differences. The first difference is that the CO fuel effects are not a ratio to VOC emissions. Instead, the fuel effects for a given target fuel are a ratio to a base reference fuel whose fuel adjustment is defined as one. This reference fuel is the fuel(s) that best represent(s) the test conditions at the Arizona IM lane where the primary emission factor data were acquired. See Section 2.1 and Table 2-1 for more details on the base / reference fuels. The second difference is the use of the Complex model only to compute the emission effect contributions from the non-sulfur fuel parameters. For CO, a separate fuel sulfur model (MOBILE6 Sulfur Model (M6SM)) is applied to compute the fuel sulfur effects after the basic complex model calculations are done (see Section 5.0 - Fuel Sulfur Model).

3.1 Carbon Monoxide Complex Model Mathematical Algorithm

The Complex Model algorithm is presented in this section in a series of nine calculation steps. Each variable is defined in the steps and where possible the actual calculation coefficients (or at least a sample calculation) are provided.

Because the effects of fuel sulfur are applied in the MOVES Sulfur model, they have been removed from the CO Complex model by setting the fuel sulfur level to a dummy value of 30 ppm for all of the target fuels. This will cause the multiplicative sulfur effects to be unity. The multiplicative MOVES Sulfur model is applied subsequent to the CO Complex model.

The CO algorithm uses the same algorithm as the Complex model air toxics algorithm for Steps 1 through 6 (i.e., Section 2.2). Different values for the coefficients are used, and a different set of Excel workbooks are used to contain the coefficients and other parameters. These steps are repeated in this section with only minor name changes for the sake of the reader who only reads the carbon monoxide section. The reader who has already read Sections 2.2.1 through 2.2.6 may find this section redundant.

3.1.1 Step 1

This series of steps are used only for the carbon monoxide (CO) pollutant.

They are performed for each of the MOVES emission processes:

running,
start
extended idle / crankcase

They are performed for both the Target and Base fuels. The variable baseSumCoeff is the sum for the base fuel, and the variable targetSumCoeff is the sum for the target fuels.

$$\text{basesumcoeff} = \text{coeff1} + \text{coeff2} \quad \text{Eq 3-1a}$$

$$\text{targetsumcoeff} = \text{coeff1} + \text{coeff2} \quad \text{Eq 3-1b}$$

The calculations are performed for each fueltype (i.e., currently gasoline only), for each fuelFormulation, for each fuel model year combination and for all cmpID variables (denoted as cmpID in Table 3-1). There are up to 64 different cmpID variables that represent the effects of individual fuel parameters and cross products of fuel parameters determined from statistical analysis of the data. Most of the individual CO fuel models only use a fraction of the 64 different cmpID variables. Currently, the variable “coeff3” is not used in the calculation. It is reserved for future possible use.

Table 3-1 ComplexModelParametersCO		
Fields	Datatype	Description
polProcessID	smallint(6)	PK: standard polProcessID variable
fuelModelID	smallint(6)	PK: basic fuel and technology model index
cmpID	smallint(6)	PK: all fuel property variable
coeff1	float	First order coefficients used in calculations
coeff2	float	Second order coefficients used in calculations
coeff3	float	Third order coefficients (placeholder) used in calculations.

3.1.2a Step 2a

In this Step 2a, the baseSumCoeff variable computed in Step 1 along with two new variables “baseValue” and “centeringValue” are used to calculate a subsequent variable BaseProd. This calculation is performed only for the ‘base’ fuel (an analogous calculation is performed for the target fuel). Like Step 1 this calculation is performed for each pollutant / process / fuel-type / fuelformulationID (base only) / fuelModelID and cmdID combination. Mathematically, the equation is given by Eq 3-2a.

$$\text{Baseprod} = \text{basesumcoeff} * (\text{baseValue} - \text{centeringValue}) \quad \text{Eq3-2a}$$

The variable “baseValue” is found in Table 2-1 for all of the parameters. The table MeanFuelParametersCO has the following structure as used in MOVES.

```

fueltypeid
modeleargroupid
fuelparameterid
fuelparametername
basevalue
centeringvalue

```

The baseValue variable is the particular fuel parameter cmpID for the base fuel (i.e., sulfurlevel, RVP, E200, etc). The calculation is performed separately for each fuel parameter. The “centering value” is a mean value variable used in the calculations. It was determined as part of the original statistical analysis of the data using a mixed model regression.

In some cases for the Base fuel, a particular cmdID may include a baseValue fuel parameter which is a product of two fuel parameters such as oxygen and RVP. This special case is illustrated in Eq3-2b for a baseprod that is a function of oxygen and RVP.

$$\text{Baseprod} = \frac{\text{basesumcoeff} * (\text{Oxygen} - \text{Oxygen centering value}) * (\text{RVP-RVP centering value})}{\text{RVP-RVP centering value}} \quad \text{Eq3-2b}$$

Table 3-2 MeanFuelParameters		
Fields	Datatype	Description
polProcessID	smallint(6)	PK: standard polProcessID variable
fuelTypeID	smallint(6)	PK: fuelTypeID = 1 only
modelYearGroupID	int(11)	PK: two new mygIDs added
fuelParameterID	Smallint(6)	PK: major fuel property variable
baseValue	float	Baseline fuel properties. Compared to Arizona fuel parameters for HC, CO and NO _x .
centeringValue	float	Fuel parameter mean value used in calculations.
stdDevValue	float	Fuel parameter standard deviation used only in HC and NO _x calculations.

3.1.2b Step 2b

In this step 2b, the targetSumCoeff variable (calculated in Step 1) along with the variables “fuelParameter” and “centeringValue” are used to calculate a subsequent variable TargetProd. This calculation is performed only for each of the target fuels which are being evaluated. Like Step 1 this calculation is performed for each pollutant / process / fuel-type / fuelformulation (target fuels only) / fuelModelID and all possible cmdID combinations. Mathematically, the equation is given by Eq 3-3a. The fuelparameter variable is the particular fuel parameter for the target fuel (i.e., sulfurlevel, RVP, E200, etc) that the user wishes to evaluate. The calculation is performed separately for each fuel parameter.

$$\text{Targetprod} = \text{targetSumCoeff} * (\text{fuelparameter} - \text{centerValue}) \quad \text{Eq 3-3a}$$

In some cases for the Target fuel, a particular cmdID may include a fuel parameter which is a compounding of two fuel parameters such as oxygen and RVP. This special case is illustrated in Eq3-3b for a Targetprod that is a function of oxygen and RVP.

$$\text{Targetprod} = \frac{\text{Targetumcoeff} * (\text{Oxygen} - \text{Oxygen centering value}) * (\text{RVP-RVP centering value})}{\text{RVP-RVP centering value}} \quad \text{Eq3-3b}$$

3.1.3 Step 3

In this step the variables eBaseProdSum and eTargetProdSum are calculated for each pollutant, process, fuelTypeID, fuelformulationID (base and target), and fuelModelID combination. The variables eBaseProdSum and eTargetProdSum are the exponential sum of each of the individual BaseProd and TargetProd variables. The sums are across all of the possible cmdID (1 to 64) groups.

$$eBaseprodSum = EXP [SUM(Baseprod) \text{ where cmdID} = 1 \text{ to } 64] \quad \text{Eq3-4a}$$

$$eTargetprodSum = EXP [SUM(Targetprod) \text{ where cmdID} = 1 \text{ to } 64] \quad \text{Eq3-4b}$$

In cases where the SUM(Baseprod) or SUM(Targetprod) equals zero, the value of eBaseprodSum or eTargetprodSum is set to zero rather than calculated as unity.

4.1.4 Step 4

In this step the variable Ratio1 is calculated for each pollutant, process, fuelTypeID, fuelModelID, fuelformulationID (the unchanging base fuel and variable target fuel) and fuelModelID combination using Equation 3-5. There are ten fuelModelID's for the carbon monoxide model.

$$\text{Ratio1} = \left(\frac{eTargetprodSum}{eBaseprodSum} \right) - 1.0 \quad \text{Eq3-5}$$

3.1.5 Step 5

In this step, the variable Ratio2 is computed by multiplying Ratio1 by a fuelModelWtFactor variable. Each of the ten fuel models has an associated weighting factor which is a function of ageID (31 years) and two broad model year groups (1960-2000 and post-2000). The structure of the table is shown in Table 3-3, and the names of the individual fuel models are provided in Table 3-4. The individual fuelmodelID's represent fuel metering, EGR, catalyst and air injection technology groupings, and the weighting factors provide a relative weighting between these groups. The weighting factors which are used in MOVES are different from those used in the original Complex model. They now vary by model year group because of the changing important of technology groupings (the original does 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). The fuelmodelID weighting factors now weight the models according to vehicle age. With fuelmodel=10 getting a weighting (based on MOBILE6.2 – MOVES does not contain the concept of "High" and "Normal" emitters) that ranges for 0.01 percent at age zero to 32.8 percent at 30 years.

Table 3-3 FuelModel Weighting Factors

Fields	Datatype	Description
fuelModelID	smallint(6)	PK: basic fuel and technology model index
modelYearGroupID	int(11)	Only two groups
ageID	smallint(6)	Age 0 through 30
fuelModelWtFactor	float	Weight factor that sums to unity for each fuelModelID and modelYearGroupID

Table 3-4 FuelModel Names

Fuel Model ID	Fuel Model Name
1	PFI & 3way & No Air & EGR
2	PFI & 3way & No Air & No EGR
3	TBI & 3way & No Air & EGR
4	PFI & 3way+Ox & Air & EGR
5	PFI & 3way & Air & EGR
6	TBI & 3way & Air & EGR
7	TBI & 3way+Ox & Air & EGR
8	TBI & 3way & No Air & No EGR
9	CARB & 3way+Ox & Air & EGR
10	All High Emitters
11	All Tier2

$$\text{Ratio2} = \text{Ratio1} * \text{fuelModelWtFactor} \quad \text{Eq3-6}$$

Similar to the air toxics model, model #11 - the All Tier2 model is not part of the calculation and receives a weighting of zero.

3.1.6 Step 6

In this step, the Ratio2 variables are summed across the ten fuel models. This produces the variable CODifferenceFraction. It is a weighted sum of all of the fuel models and the base and target fuel effects. In essence, it is the fractional difference in

CO emissions between the base and target fuels. It is calculated for each combination of pollutant, process, fuel type, age and fuel formulation.

$$\text{CODifferenceFraction} = \frac{\sum_{i=1}^{\max(\text{fuelmodels})} \text{Ratio2}_i}{\text{fuelmodel}[\text{max}(\text{fuelmodels})]} \quad \text{Eq3-7}$$

$$\text{fuelmodel}[\text{max}(\text{fuelmodels})] = 10 \quad \text{for carbon monoxide}$$

3.1.7 Step 7

This step differs from the air toxics algorithm described in Section 2. The non sulfur fuel effects on CO emissions are contained in the CODifferenceFraction variable. By definition, the Base fuel is the fuel formulation that was generally available in the State of Arizona during the period where EPA primary test data were collected on carbon monoxide emissions. Since sulfur effects are not included in this model only the low sulfur (30 ppm sulfur) reference - base fuel A (see Table 2-1) may be used as the Base fuel. The target fuel is the fuel which is to be evaluated. The variable CODifferenceFraction computed in Eq3-8 contains the fractional emission difference between the target and the base fuels.

$$\text{COFuelEffectNoSulfur} = 1.0 + \text{CODifferenceFraction} \quad \text{eq3-8}$$

Eq3-8 calculates the CO fueladjustment factor without sulfur. This algorithm is used only for the processes of running and start and for the CO pollutant, and is used only for gasoline fueled vehicles. It is computed for each age, fuel formulation and model year group (MOVES contains two distinct model year groups with different base sulfur levels).

3.1.8 Step 8

Apply the MOBILE6 Sulfur Model (M6SM) to CORatioNoSulfur to compute the final CO FuelAdjustment Factor which is used to correct the CO emission factors in MOVES for gasoline fuel effects. The details on the M6SM model are shown in Section 5.0 and the process for combining the sulfur and non sulfur fuel models is shown in Section 6.0.

4.0 Predictive Model Algorithms for Total Hydrocarbon and Nitrogen Oxide Fuel Effects

4.1 Predictive Model Overview

The MOVES model uses the Predictive Model to simulate the effect of gasoline fuel parameters on hydrocarbon (HC) and nitrogen oxide (NO_x) emissions. The HC and NO_x Predictive Models utilize two base fuels (30 ppm Sulfur and 90 ppm Sulfur). The 30 ppm fuel is the base fuel for 2001-and-later model years, and 90 ppm sulfur is the base fuel for 1975 through 2000 model years. The remaining fuel parameters are identical between the two base fuels (see Table 2-1).

The Predictive Model effects from all fuel parameters are applied to 1960 through 1993 model years. The effects are not applied for model years 2004-and-later (Tier2-and-later emission standards). This means that in MOVES2010a, for 2004-model-year-and-later gasoline vehicles, exhaust HC and NO_x emissions are insensitive to all fuel parameters (vapor pressures, aromatic contents, distillation fractions, etc.), EXCEPT for the fuel sulfur level parameter.

The decision to apply no Predictive Model effects for 2004-and-later model years in MOVES2010 is based on limited test evidence, and on engineering judgment that the advanced combustion and emission control technologies used in Tier2-and-later gasoline vehicles are likely to be insensitive to most fuel parameters (other than sulfur). However, the EPA test program and analysis are designed to provide data on this question.

Since the release of MOVES2010a, EPA test and statistical analysis on 2004 and later model years has shown that virtually all of the pollutants (criteria and air toxic) are sensitive to a full array of fuel parameters – not just fuel sulfur. Consequently, the assumption of ‘insensitivity’ to fuel parameters now used in MOVES2010a will be substantially changed in future versions of the MOVES model.

4.2 Predictive Model Step 1

The overall goal of the Predictive model algorithm is to develop a multiplicative fuel correction factor for a given fuel formulation which can be applied to the base emission rates (BaseE) as calculated by MOVES. This is shown mathematically in the simple Equation 4-1.

$$\text{Fuel Corrected Emissions} = \text{Fuel Correction} * \text{Sulfur Correction} * \text{BaseE} \quad \text{Eq 4-1}$$

The Fuel Correction shown in Eq 4-1 is the ratio between the Predictive model output for the Target fuel and the Predictive model output for Base fuel. This is shown in Equation 4-2

$$\text{Fuel Correction} = \text{PredictiveModel}\{\text{Target}\} / \text{PredictiveModel}\{\text{Base}\} \quad \text{Eq 4-2}$$

Where Target is the emissions using the Target fuel formulation and Base refers to emissions with the Base fuel formulation. The same algorithms are used for both the Target and Base Predictive model calculations. The only difference between the two calculations is the different fuel properties for the Target fuel and the Base fuel.

4.3 Predictive Model Step 2

The Predictive model is a series of statistically derived fuel and emission models. During the analysis process, several models were developed but only three models were chosen for HC, and six models were chosen for NOx. For a given pollutant, each model is equally weighted for the computation of the final result. Table 4.1 lists the individual models.

Table 4-1 MOVES Fuel Model Naming Conventions		
Model Number	HC	NOx
1	107	302
2	108	303
3	112	304
4		305
5		306
6		307

Each of the fuel models (three for HC and six for NOx) are function of 19 fuel parameters and combinations (products) of fuel parameters. All of the models have the same list of parameters. However, some models have coefficients of zero for certain parameters. The parameters are listed in Table 4-2 contains a complete list of all of the Predictive model parameters and equations. In the MOVES algorithm the “Intercept” and “HI” terms are set to unity.

Table 4-2 Fuel Parameters for the Predictive Models

Parameter Number	Fuel Parameter(s)
1	Intercept
2	RVP
3	T50
4	T90
5	AROM
6	OLEF
7	OXYGEN
8	SULFUR
9	HI
10	T90*T90
11	T50*T50
12	T90*OXY
13	SUL*HI
14	OXY*OXY
15	T90*ARO
16	T50*HI
17	OLE*OLE
18	T90*OLE
19	ARO*ARO

The first step in applying the model is to create a normalized fuel parameter (N_Parameter) as shown in Equations 4-3a and 4-3b. It is performed for each of the parameters listed in Table 4-2, for each of the three HC models or each of the six NO_x models, and for both the Target and Base fuels.

$$N_Parameter = \frac{(\text{fuelParameter} - \text{centeringValue})}{\text{stdDevValue}} \quad \text{Eq 4-3a}$$

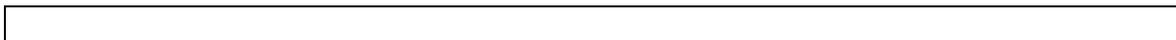
Where:

fuelParameter - is the particular fuel parameter value of either the target or base fuel (i.e., RVP(psi)). The values for the Target and Base fuels are taken from the MOVES Fuel Formulation table.

The related Equation 4-3b is used for a compound term (i.e., T90*OLE)

$$N \text{ Parameter} = \frac{((T90 - \text{centeringValue}) / \text{stdDevValue}) * ((\text{Olefin} - \text{centeringValue}) / \text{stdDevValue})}{\text{stdDevValue}} \quad \text{Eq4-3b}$$

CenteringValue and the stdDevValue are fuel parameter constants. These are shown in Table 4-3.



**Table 4-3
MOVES Predictive Model Centering Values and StdDev Values**

		Standard
Term	Mean	Deviation
RVP	8.51	0.781459
T50	205.62	17.612534
T90	310.65	20.869732
AROM	27.64	6.561886
OLEF	6.93	5.143184
OXYGEN	1.49	1.249356
SULFUR	183.14	143.055894

4.4 Predictive Model Step 3

In this step the normalized fuel parameter from Eq 4-3a and Eq 4-3b are multiplied by the variable “coeff1” for each of the each of the parameters (i) listed in Table 4-2, for each of the fuel models (i.e., HC has three and NOx has six), and for both the Target and Base fuels. This produces a matrix of products for both the Target and Base fuels. The values for the variable coeff1 are shown in the attached spreadsheet PredictiveModelCoefficients.xls.

$$\text{Product (i)} = \text{N Parameter} * \text{coeff1(i)} \quad \text{Eq 4-4}$$

4.5 Predictive Model Step 4

For each of the fuel models, and the Target and Base fuel formulations the values of Product(i) are summed across the 19 fuel parameters listed in Table 4-2. The Exponent of the sums is calculated.

$$\text{ModelResult(j)} = \text{EXP} [\text{SUM}(\text{Product}(i,j)) \quad i = 1, 19] \quad \text{Eq 4-5}$$

Where (i) is the fuel parameter and (j) is the fuel model.

4.6 Predictive Model Step 5

In this step the ModelResult calculated in Step 4 for each fuel model (three HC models and six NOx models) are weighted (averaged) together. This operation is done for both the Target and Base fuels to produce the variable “WeightedResult”. For both HC and NOx, each of the fuel models is equally weighted.

$$\text{WeightedResult}[\text{target}] = \sum[\text{fuelModelWtFactor} * \text{ModelResult}(j)] \quad \text{Eq 4-6}$$

$$\text{WeightedResult}[\text{base}] = \sum[\text{fuelModelWtFactor} * \text{ModelResult}(j)] \quad \text{Eq 4-7}$$

Where (j) is three for HC and (j) is six for NOx.

4.7 Predictive Model Step 6

We next calculate the Fuel Correction variable shown in Equation 4-1 and 4-2. This is the fuel adjustment factor **WITHOUT** the effects of sulfur. In MOVES it is computed for each emission process (running and start), each target fuel formulation which is being evaluated, each model year group / age group and each source type.

$$\text{Fuel Correction} = \text{WeightedResult}[\text{target}] / \text{WeightedResult}[\text{base}] \quad \text{Eq 4-8a}$$

By definition, for Tier2-and-later model years the Fuel Correction variable is set to one for all non sulfur effects. Since there are no sulfur effects in this algorithm Equation 4-8b is used.

$$\text{Fuel Correction} = 1.0 \quad \text{Eq 4-8b}$$

4.8 Predictive Model Step 7

In this step the Sulfur Correction factor is applied to Fuel Correction variable calculated in Eq 4-8a or Eq 4-8b. The Sulfur Correction factor is computed by applying the MOBILE6 Sulfur Model (M6SM). The details on the M6SM model are shown in Section 5.0 and the process for combining the sulfur and non sulfur fuel models is shown in Section 6.0.

5.0 Fuel Sulfur Model

5.0 Fuel Sulfur Model Background

In the MOVES application of the Complex and Predictive Models, the emission effects of fuel sulfur were removed and the multiplicative correction factors for sulfur were set to one. Instead of using the sulfur effects from these two models, the fuel sulfur effects from the MOBILE6.2 Fuel Sulfur Model (M6Sulf) were applied to both start and running emissions for HC, CO and NO_x emissions for all model years (*the exception is the final sulfur adjustment factor for pre-1975 model years which is unity, ie. no adjustment*). In MOVES2010a, the Tier2 (2004 and later model years) utilize the M6Sulf model, but this assumption will likely be reviewed once substantial emission / fuel data is available from the EPA testing.

Two issues become apparent when applying the M6Sulf effects in the MOVES model. These are: (1) The MOBILE6.2 model contains separate effects for High and Normal emitters, but MOVES does not classify emissions or vehicles according to these terms. (2) The MOVES model needs to model Tier2 vehicles using low sulfur fuel (i.e., < 30 ppm sulfur). However, the MOBILE6.2 sulfur factors are based entirely on pre-Tier2 vehicles operating on sulfur levels of 30 ppm or higher.

In MOBILE6.2, different fuel sulfur effects (coefficients) and equations (i.e., log-log and log-linear) were used for High and Normal emitters (*a “High” emitter was defined as a vehicle which emitted twice its applicable HC or NO_x standard or three times its CO standard*). MOBILE6.2 computes emission rates for High and Normal emitters separately and weights them according to a complex algorithm that is built into the model. However, in general the weighting between High and Normal emitters was frequently about equal for the typical vehicle on the road (new vehicles had lower rates of high emitters, though). For the MOVES sulfur effect, a straight arithmetic average between the High and Normal effects was calculated and used for consistency with the MOBILE6 approach.

For some of the late model year vehicles (2001 – 2003), this approach may model these vehicles to be less sensitive to sulfur than more recent data from 2004+ model year – Tier2 vehicles would suggest. This is because (1) the distribution of “high” emitters in the fleet is smaller (< 50%) than it has been historically – although, their emission contribution is probably still very significant, and (2) the “high” emitter corrections are typically log-linear relationships and less sensitive to sulfur than the log-log “normal” emitter corrections.

To model very low sulfur fuels in MOVES, we extrapolated the MOBILE6 emission / fuel sulfur relationship to fuels below 30 ppm sulfur. Since some of these relationships are log-log in structure, such an extrapolation could lead to meaningless results. To prevent highly non-linear relationships which are inherent in log-log mathematics from dominating the MOVES emission results, a fuel adjustment ‘floor’ of 0.85 was placed in the code. This ‘floor’ prevents MOVES from reducing the emission

rate by more than 15 percent from its ‘base’ emission rate as a result of changing base fuel formulation (30 ppm sulfur) to some other lower level (i.e., 0.01 ppm sulfur). This floor should prevent the most asymptotic portion of the log-log relationship from being utilized.

As a final thought on this topic, EPA realizes the inherent problems associated with using these out of date fuel relationships on Tier2 and later vehicles operating on low sulfur fuels. As such, EPA plans to revise them as soon as sufficient new data are collected and analyzed as part of the EPAct test program.

5.1 MOBILE6 Sulfur Algorithm in MOVES

In MOVES, the M6Sulf model data are stored as a set of equation coefficients in a database table. It has the following table structure:

pollutantID
processID
fuelMYGroupID
M6emitterID
SourceTypeID
SulfurFunctionID
SulfurCoefficient

The M6emitterID is designated as either “Normal” or “High” and the SulfurFunctionID is designated as either “Log-Log” or “Log-Linear”. The “Log-Log” designation refers to a model with a natural log – natural log form and the “log-linear” refers the natural log-linear model.

The M6Sulf algorithm as programmed into the MOVES model contains four separate fuel sulfur models. This document and section details the algorithms in the MOVES model. It also discusses the minor changes and assumptions that had to be made to fit the MOBILE6 algorithms into the MOVES structure. The reader who is interested in the primary development of these fuel models needs to refer to the primary documentation in the EPA report EPA420-R-01-039 “Fuel Sulfur Effects on Exhaust Emissions – Recommendations for MOBILE6” by Venkatesh Rao. The internet link is:

<http://www.epa.gov/otaq/models/mobile6/r01039.pdf>

The individual models which are used in the MOVES model are:

Short Term Sulfur model
Long Term Sulfur model
Sulfur Irreversibility model
Sulfur GPA model

In addition, space is reserved in the MOVES model to incorporate a new fuel sulfur model for Tier2 (2004-and-later model year vehicles) if and when it become available.

5.2 Short Term Sulfur Effects

The Short Term Sulfur Effects is an adjustment to the base emissions as a function of the sulfur volume of the gasoline in parts per million. The calculations begin by using Equations 5-1a and 5-1b. These are used in cases where the log-log relationship is required (the variable SulfurFunctionID is set to 'log-log'. This is for Tier0 and LEV+ vehicles. The variable “sulfShortTarget” is the correction factor for the sulfur level of the fuel which is being modeled. SulfShort30 is the correction factor for the basis sulfur (table SulfurBase. sulfurBasis variable) level. The sulfur basis is always 30 ppm – even for model year groups which use 90 ppm Sulfur as the baseline. A 90 ppm sulfur base fuel will not have a SulfShortAdj that is equal to 0.0.

$$\begin{aligned} \text{sulfShortTarget} &= \text{EXP}(\text{sulfurCoeff} * \text{LN}(\text{sulfur})) && \text{Eq 5-1a} \\ \text{sulfShort30} &= \text{EXP}(\text{sulfurCoeff} * \text{LN}(\text{sulfurBasis})) && \text{Eq 5-1b} \end{aligned}$$

The Short Term Sulfur effects for Tier1 vehicles (i.e. model years 1994-2000}) use a log-linear algorithm as in equations 5-2a and 5-2b. Again the base fuel sulfur is 30 ppm. High emitters may use a different equational form (i.e, log-log) in some cases. The “Sulfur Model Coefficients.xls” workbook in the variable SulfurFunctionID shows which form of the equation is used.

$$\begin{aligned} \text{sulfShortTarget} &= \text{EXP}(\text{sulfurCoeff} * (\text{sulfur})) && \text{Eq 5-2a} \\ \text{sulfShort30} &= \text{EXP}(\text{sulfurCoeff} * (\text{sulfurBasis})) && \text{Eq 5-2b} \end{aligned}$$

The Short term sulfur effect (SulfAdj) for all groups is computed using Eq 5-3.

$$\text{SulfShortAdj} = (\text{SulfShortTarget} - \text{SulfShort30}) / \text{SulfShort30} \quad \text{Eq 5-3}$$

5.3 Calculate Long Term Sulfur Effects

The long term sulfur effects account for sulfur exposure over several thousand miles of driving. They values used in MOVES are stored in the sulfurLongCoeff variable in the MOVES table M6SulfurCoeff. The values for sulfurLongCoeff are a function of pollutant. They are:

HC	2.50
CO	2.36
NOx	1.47

These effects are multiplied by the short term sulfur effects calculated above in Eq 5-3 to produce the variable sulfAdj2. Sulfur levels of 30 ppm or less are assumed to have no Long Term effects.

$$\text{sulfAdj2} = \text{SulfShortAdj} * \text{sulfurLongCoeff} \quad \text{Eq 5-4}$$

5.4 Calculation of the Sulfur Irreversibility Effects

In this step, the average emission effects of sulfur which cannot be reversed if exposure is recorded are computed. They apply to only Tier2 (2004+ model years vehicles only), and apply only to Target fuel sulfur levels which are greater than 30 ppm sulfur. Fuel sulfur levels less than or equal to 30 ppm do not cause such effects to occur. The same effects are applied to all three pollutants (HC, CO and NOx) and processes (start and running). The SulfurCap is a function of model year group.

<u>Model Year Group</u>	<u>SulfurCap</u>
2004 – 2005	303 ppm sulfur
2006 – 2007	87 ppm sulfur
2008 +	80 ppm sulfur

If the fuel sulfur level is greater than 30 ppm but less than the SulfurCap, Equation 5-5a is used to compute the SulfIRR effects, and the effect is applied as a function of model year group.

If sulfur < sulfurCap

$$\text{SulfIRR} = \text{EXP} (\text{sulfurCoeff} * \text{LN}(\text{sulfurCap})) \quad \text{Eq 5-5a}$$

Eq5-5b computes the sulfur irreversibility effects if the selected sulfur level is greater than the maximum sulfur level. Sulfur levels above the SulfurCap are not expected in normal use of the MOVES model.

If sulfur > sulfurCap

$$\text{SulfIRR} = \text{EXP} (\text{sulfurCoeff} * \text{LN}(\text{sulfur})) \quad \text{Eq 5-5b}$$

5.5 Putting the Short, Long and Irreversibility Sulfur Effects Together

Equation 5-7 puts all of the sulfur effects together into the final fuel sulfur effects. It is labeled as sulfAdj3. This variable contains the short term, long term and irreversible effects together. Equation Eq5-6 calculates the intermediate sulfMax variable.

$$\text{sulfMax} = (\text{SulfIRR} - \text{sulfShort30}) / \text{sulfShort30} \quad \text{Eq 5-6}$$

Where

SulfIRR is from Eq 5-5a or Eq 5-5b.
sulfShort30 is from Eq5-1b or Eq5-2b

$$\text{sulfAdj3} = 1.0 + [\text{IRFactor} * \text{sulfMax} + (1.0 - \text{IRFactor}) * \text{sulfAdj2}] \quad \text{Eq 5-7}$$

Where

sulfAdj2 is the result of Eq5-4

IRFactor is equal to 0.425.

To prevent the log-log based sulfur corrections from rapidly approaching zero as the sulfur levels approach zero, the following limit is placed.

$$\text{sulfAdj3} = 0.85 \quad \text{Where } \text{sulfAdj3} \leq 0.85 \quad \text{Eq 5-8}$$

5.6 Sulfur GPA Effects

During the years 2004-2006, gasoline sulfur levels in the Sulfur “Geographical Phase-In Area” (Sulfur GPA) were allowed to be higher than elsewhere in the nation. MOVES accounts for this with the Sulfur GPA Effects. The algorithm applies a maximum sulfur exposure of 330 ppm sulfur to areas that are GPA areas. The GPA areas are mostly Rocky Mountain areas and are identified in the county table of the MOVES2010 database.

In this step (Eq 5-9) the sulfurGPA effects are calculated for both Normal and High emitter groups. Sulfur GPA is only applied to model years 2004, 2005 and 2006, and for fuel sulfur levels which are greater than 30 ppm sulfur. It is also limited to GPA areas, and is a sulfur phase-out strategy. In all other cases GPAsulfAdj is equal to the regular sulfur adjustment, and no additional GPA effect is applied in the MOVES model. SulfurGPA uses the same basic algorithm as the regular sulfur adjustment, except the variable SulfurBase. The sulfurGPAMax (330 ppm sulfur) is substituted in the equation in place of the actual sulfur level of the fuel to be evaluated. The value of 330 ppm is a typical worse case GPA scenario sulfur level.

$$\text{sulfGPA1} = \text{EXP} (\text{sulfurCoeff} * \text{LN}(\text{sulfurGPAMax})) \quad \text{Eq 5-9}$$

$$\text{SulfGPA} = (\text{sulfGPA1} - \text{sulfShort30}) / \text{sulfShort30} \quad \text{Eq 5-10a}$$

For NOx High emitters the numerator (sulfGPA1 and sulfShort30) is multiplied by 0.60.

$$\text{sulfGPA} = \text{SulfGPA} * \text{sulfurLongCoeff} \quad \text{Eq 5-10b}$$

$$\text{GPASulfadj} = 1.0 + [\text{IRFactor} * \text{sulfGPA} + (1.0 - \text{IRFactor}) * \text{sulfAdj2}] \quad \text{Eq 5-11a}$$

Where

sulfAdj2 is the product of Eq5-4

IRFactor is equal to 0.425.

In non GPA years, or in areas where sulfur < 30 ppm, Eq 5-11b is used. It is also used in cases if the sulfur level is greater than sulfurGPAMax (i.e., 330 ppm). As a general rule, the GPASulfadj can NEVER be smaller than sulfAdj3, and the two are equal most of the time.

$$\text{GPASulfadj} = \text{sulfAdj3} \quad \text{Eq 5-11b}$$

The GPASulfadj is applied in the model by weighting it by the fraction of GPA is a particular county. In the default cases, this fraction is always zero or one. However, GPA fraction is a user input, so alternative values between zero and one may be entered as inputs.

$$\text{Final Sulfur Adj} = \text{SulfAdj3} * (1 - \text{GPAFraction}) + \text{GPASulfadj} * \text{GPAFraction} \quad \text{Eq 5-12}$$

5.7 Normal and High Emitter Correction Factor Weighting

As discussed in general in Section 5.0, the M6Sulf algorithm produces a sulfur correction for both “Normal” and “High” emitters. Since MOVES does not define vehicles as “Normal” and “High” emitters in terms of emissions rates, the sets of model coefficients were regarded as independent models and equaled weighted for consistency with the MOBILE6 model. The variable wtHigh is set equal to 0.50.

$$\text{sulfAdj3(Target)} = (1-\text{wtHigh}) * \text{sulfAdj3(normal)} + \text{wtHigh} * \text{sulfAdj3(high)} \quad \text{Eq 5-13a}$$

$$\text{sulfAdj3(Base)} = (1-\text{wtHigh}) * \text{sulfAdj3(normal)} + \text{wtHigh} * \text{sulfAdj3(high)} \quad \text{Eq 5-13b}$$

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

$$\text{GPAsulfAdj3(Target)} = (1-\text{wtHigh}) * \text{GPASulfadj (normal)} + \text{wtHigh} * \text{GPASulfadj (high)} \quad \text{Eq 5-14a}$$

$$\text{GPAsulfAdj3(Base)} = (1-\text{wtHigh}) * \text{GPASulfadj (normal)} + \text{wtHigh} * \text{GPASulfadj (high)} \quad \text{Eq 5-14b}$$

5.9 Computing the Sulfur Adjustment for the Base Fuels.

Sections 5-2 through 5-7 must be repeated and applied for the two base fuels of 90 ppm sulfur and 30 ppm sulfur corresponding to the two model year groups (1960-2000 and 2001-2050), respectively. This is because the final sulfur fuel adjustment (see Eq 5-15) factor is the ratio of the Target fuel adjustment and its Base fuel adjustment. The M6Sulf model calculations for the Base fuel are exactly the same as those presented in the sections above and are not repeated here. All other properties of these fuels are held constant for the sulfur correction. The Final fuel sulfur correction for the 30 ppm case is one because the base fuel of 30 ppm sulfur is equal to the 30 ppm sulfur basis. The 30 ppm sulfur level is called the basis (i.e., sulfShort30 variable) because the entire MOBILE6.2 Fuel Sulfur algorithm was developed based on this level. The calculation result is not one for the 90 ppm base sulfur.

$$\text{FinalSulfAdj} = \text{sulfAdj3(Target)} / \text{sulfAdj3(Base)} \quad \text{Eq 5-15}$$

Where sulfAdj3 is the sulfur adjustment from Sections 5.2 through 5.8 and the sulfAdj3(base) is the sulfur adjustment for either the 30 ppm or 90 ppm sulfur base (or reference) cases.

The calculation is similar for the GPA case (Eq 5-16).

$$\text{FinalGPASulfAdj} = \text{GPASulfadj (Target)} / \text{GPASulfadj(Base)} \quad \text{Eq 5-16}$$

6.0 Combining the Predictive and Complex Model with the Sulfur Model

This section describes how the fuel adjustment factors generated by the Predictive and Complex model without sulfur effects are combined with the fuel adjustment factors generated by the M6Sulf model in Section 5.0. This combination is done only for pollutants HC, CO and NO_x. The air toxic pollutants do not use the M6Sulf model (i.e., the air toxics CM model contains sulfur effects).

Since all three of these models produce multiplicative correction factors the final combination of the two factors is multiplicative. The general equation is shown in Eq 6-1.

$$\text{MOVES Fuel Adjustment} = \text{Non Sulfur Fuel Adjustment} * \text{M6Sulf Adjustment} \quad \text{Eq 6-1}$$

6.1 Overall Fuel Adjustment for Model Year 1960 through 1974 Vehicles.

In the case of all 1960 through 1974 vehicles, the Overall Fuel Adjustment is set to one. This was done because little or no data are available for these model years and most of the vehicles do not contain a catalytic converter or modern electronic fuel / engine management components which would be sensitive to changes in fuel composition.

$$\text{FuelAdjustment} = 1.0 \quad \text{Eq 6-2}$$

6.2 Overall Fuel Adjustment for Model Year 1975 through 2003 Vehicles.

The Overall Fuel Adjustment for HC, CO and NO_x pollutants for 1975 through 2003 model year vehicles is the product of the final fuel adjustments calculated with the Complex or Predictive models (i.e., COFuelEffectNoSulfur or Fuel Correction (Eq 4-8a), and the FinalSulfAdj calculated in the M5Sulf model.

$$\text{FuelAdjustment} = \text{finalSulfAdj} * \text{RatioNoSulfur} \quad \text{Eq 6-3}$$

Where

*Model Year >= 1975 and Model Year <= 2003 and Pollutant in (HC, NO_x) or
Model Year >= 1975 and Pollutant in (CO)*

6.3 Overall Fuel Adjustment for Model Year 2004 and Later Vehicles.

The Overall Fuel Adjustment for HC and NO_x pollutants for model year 2004 and later model year vehicles is the Final Sulfur Adjustment computed by the M6Sulf model. It contains only fuel sulfur effects.

$$\text{FuelAdjustment} = \text{finalSulfAdj} \quad \text{Eq 6-4}$$

Where
Model Year >=2004 and Pollutant in (HC, NO_x)

6.4 Overall fuelAdjustmentGPA for Model Years 2004 Through 2006

In this step the fuelAdjustmentGPA is set to the final value for use in the MOVES.

$$\text{fuelAdjustmentGPA} = \text{FinalGPASulfAdj} \quad \text{Eq 6-5}$$

Where
Modelyear in (2004, 2005, 2006) and finalGPASulfAdj < 1.0;

$$\text{fuelAdjustmentGPA} = \text{fuelAdjustment} \quad \text{Eq 6-6}$$

for all other cases

7.0 Biodiesel Fuel Effects

The Draft MOVES2009 version released in April 2009 contains diesel fuel parameters and emission effects only for diesel fuel sulfur level (ppm sulfur in the fuel). This parameter is used in a fuel-sulfur mass balance equation to calculate sulfate PM emission levels, and was expanded in MOVES2010 to include gaseous SO₂ emissions. The fuel sulfur mass balance methodology was taken from EPA PART5 / MOBILE6.2 model and is fully documented in the MOBILE6.2 documentation. See the link:

<http://www.epa.gov/oms/models/mobile6/m6tech.htm>

New sulfate (SO₄) and sulfur dioxide (SO₂) emission factors were also developed for MOVES2010a for gasoline vehicles. The data were obtained from a set of about 30 vehicles in the EPA Kansas City test program in which both fuel sulfur measurements and SO₄ particulate measurements were made. See the document “Development of Gasoline and Diesel Vehicle Sulfate and Sulfur Dioxide Emissions for the MOVES Model”. The sulfate and sulfur dioxide emissions for diesels and pre-1980 gasoline model years were unchanged from MOBILE6.2

MOVES2010 contains an additional parameter called BioDieselEsterVolume. It represents the percentage of biodiesel ester by volume in a Target fuel. Currently all entries in the default fuel supply for MOVES2010 are NULL and the model performs no biodiesel calculations. However, users could enter local information about biodiesel fuels.

Mathematically, the BioDieselEsterVolume variable is used with the BioDiesel Fuel Adjustment Factors (*presented in Table 7-1*). Together these two parameters produce an overall diesel Fuel Adjustment factor for biodiesel fuels. These fuel adjustment factors (shown as percentages) give the relative increase or decrease in emissions as the result of adding biodiesel to standard on-road diesel fuel. The equation for calculating the BioDiesel adjustment factor is shown in Eq 7-1. Analogous to the gasoline fuel adjustment, the BioDiesel factor gets multiplied by the base emission rate of standard diesel vehicles.

$$\text{FuelAdjustment factor} = 1.0 + (\text{BiodieselEsterVolume}/100.0) * \text{BioDieselFactor} \quad \text{Eq 7-1}$$

The Biodiesel Fuel Adjustment factors are shown in Table 7-1.

**Table 7-1
Biodiesel Fuel Adjustment Factors as a Function of Pollutant**

Pollutant Name	BioDiesel Factor
HC	-14.1
CO	-13.8
NOx	2.2
PM2.5 and PM10.0	-15.6
Benzene	-14.1
1,3 Butadiene	-14.1
Acetaldehyde	-14.1
Formaldehyde	-14.1
Naphthalene	-15.6
Acrolein	-14.1

The individual pollutant impacts of biodiesel (B20) listed in Table 7-1 are relative to conventional diesel fuel. For example, the -14.1 factor for HC would reduce the hydrocarbon emissions from a standard diesel fuel by 14.1 percent. The biodiesel factors were based on very limited EPA testing of such fuels. See the link below.

<http://www.arb.ca.gov/fuels/diesel/altdiesel/100519BiodieselWorkshopPresB&W.pdf>

No data were available on air toxic pollutants tested on biodiesel fuels. Consequently, biodiesel will use the same air toxic / VOC ratios as are used in the computation of emissions from vehicle operating on ordinary diesel fuels (see Section 8.0).

8.0 Toxic Emissions from Diesel Vehicles

The toxics ratios in MOVES2010 for diesel vehicles were developed well over 10 years ago, and were used in MOBILE6.2.¹⁴ These ratios are provided in Table 8-1. More extensive data are now available, including recent test data on diesel engines meeting 2007 heavy-duty emission standards.^{15,16} EPA intends to update the equations and the methodology in MOVES using these data, and release the updated version at a later date. Whereas MOBILE6.2 had separate ratios for light-duty diesel vehicles and trucks based on very limited data, MOVES2010a applies the same ratios to all diesel vehicles, heavy and light-duty.

Pollutant	Ratio Type	Ratio
Benzene	VOC	0.0108
Formaldehyde	VOC	0.0807
Acetaldehyde	VOC	0.0298
Acrolein	VOC	0.0036
Naphthalene	PM10	0.001289

The air toxic pollutants for diesels are computed using equations 8-1 and 8-2. The equations are completely analogous to the simple equations used for gasoline vehicles (see Eq 2-1).

$$\text{AT Emission (g/hr)} = \text{AT Ratio} * \text{VOC Emission (g/hr)} \quad \text{Eq 8-1}$$

$$\text{AT Emission (g/hr)} = \text{AT Ratio} * \text{PM10 Emission (g/hr)} \quad \text{Eq 8-2}$$

¹⁴ Cook, R., and E. L. Glover. 2002. Technical Description of the Toxics Module for MOBILE6.2 and Guidance on Its Use for Emission Inventory Preparation. Assessment and Standards Division, Office of Transportation and Air Quality, Ann Arbor, MI. Report No. EPA420-R-02-011. <http://www.epa.gov/otaq/m6.htm>

¹⁵ Hsu, Y., and Mullen, M. 2007. Compilation of Diesel Emissions Speciation Data. Prepared by E. H. Pechan and Associates for the Coordinating Research Council. CRC Contract No. E-75, October, 2007. Available at www.crcao.org.

¹⁶ Khalek, I., Bougher, T., and Merritt, P. M. 2009. Phase 1 of the Advanced Collaborative Emissions Study. Prepared by Southwest Research Institute for the Coordinating Research Council and the Health Effects Institute, June 2009. Available at www.crcao.org.

Hydrocarbon Speciation Factors

Table 8-1 shows a simple relationship between the various hydrocarbon species in MOVES, and their relationship to the base, total hydrocarbons (THC). As the table shows the individual hydrocarbon species differ based on the presence or absence of the hydrocarbon compounds of methane, ethane and aldehydes. The term FID HC refers to the total hydrocarbons detected by a Flame Ionization Detector (FID) instrument.

All factors used in MOVES were taken from MOBILE6.2 materials and were originally produced in 1991. No new speciation factors were developed for MOVES2010a.

PollutantID	PollutantName	FID HC	Methane	Ethane	Aldehydes
1	Total Hydrocarbons	Yes	Yes	Yes	No
79	Non Methane Hydrocarbons	Yes	No	Yes	No
87	Volatile Organic Compounds	Yes	No	No	Yes
86	Total Organic Gases	Yes	Yes	Yes	Yes
80	Non Methane Organic Gases	Yes	No	Yes	Yes

8.1 Non Methane Hydrocarbon Factors

The MOVES model calculates non-methane hydrocarbons (NMHC). The MOVES model computes this hydrocarbon species by first independently calculating THC emissions and methane emissions.

(see <http://nsdi.epa.gov/otaq/models/ngm/420p05003.pdf>).

As a result of this dependence, NMHC is ‘chained’ to both THC and methane. The NMHC calculator subtracts the resulting methane emissions from the THC emissions (mechanically in MOVES it multiples methane by negative one and adds the result). If a negative emission value for NMHC is calculated, it is set to zero. The formula for calculating NMHC is shown in Eq 8-1. This formula is used only for gasoline fuels

$$\text{NMHC} = \text{THC} - \text{Methane} \quad \text{Eq 8-1}$$

8.2 VOC Speciation Calculation

The MOVES model calculates Volatile Organic Compounds (VOC). VOC is calculated from NMHC using Eq 8-2a through 8-2d and the variables ‘speciationConstant’ and ‘oxySpeciation’ coefficients. The variable ‘volToWtPercentOxy’ is a standard chemical conversion to convert percent oxygen in the fuel from a volume basis to a weight basis for variety of oxygenated fuels. Consequently, all of the standard MOVES fuel inputs for oxygenate (i.e., ETOHVolume, MTBEVolume, etc) are in terms of a percentage of oxygen by fuel volume.

For fuels containing ethanol

$$\text{VOC} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{ETOHVolume}) \quad \text{Eq 8-2a}$$

For fuels containing MTBE

$$\text{VOC} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{MTBEVolume}) \quad \text{Eq 8-2b}$$

For fuels containing ETBE

$$\text{VOC} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{ETBEVolume}) \quad \text{Eq 8-2c}$$

For fuels containing TAME

$$\text{VOC} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{TAMEVolume}) \quad \text{Eq 8-2d}$$

For pure gasoline fuels the second term drops off and only the speciationConstant is applicable. The speciationConstant is a function of fuel model year group. The variable volToWtPercentOxy is a function of oxygenate type. The values for each oxygenate type are:

Ethanol	0.3488
MTBE	0.1786
ETBE	0.1533
TAME	0.1636

The general equation for volToWtPercentOxy in MOVES is equation 8-3e.

$$\text{volToWtPercentOxy} = \frac{(\text{ETOHVolume} * 0.3488 + \text{MTBEVolume} * 0.1786 + \text{ETBEVolume} * 0.1533 + \text{TAMEVolume} * 0.1636)}{(\text{ETOHVolume} + \text{MTBEVolume} + \text{ETBEVolume} + \text{TAMEVolume})} \quad \text{Eq 8-3e}$$

8.3 NMOG Speciation Calculation

The MOVES model calculates Non Methane Organic Gases (NMOG). NMOG is calculated from NMHC using Eq 8-3a through 8-3d and the variables ‘speciationConstant’ and ‘oxySpeciation’ coefficients. The values for the variable volToWtPercentOxy are provided in Section 8.2.

For fuels containing ethanol

$$\text{NMOG} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{ETOHVolume}) \quad \text{Eq 8-3a}$$

For fuels containing MTBE

$$\text{NMOG} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{MTBEVolume}) \quad \text{Eq 8-3b}$$

For fuels containing ETBE

$$\text{NMOG} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{ETBEVolume}) \quad \text{Eq 8-3c}$$

For fuels containing TAME

$$\text{NMOG} = \text{NMHC} * (\text{speciationConstant} + \text{oxySpeciation} * \text{volToWtPercentOxy} * \text{TAMEVolume}) \quad \text{Eq 8-3d}$$

For pure gasoline fuels the second term drops off and only the speciationConstant is applicable. The speciationConstant is a function of fuel model year group.

8.4 TOG Speciation Calculation

The MOVES model calculates Total Organic Gases (TOG). These are calculated by calculating both the NMOG emissions and the methane emissions in their respective calculators. TOG is depend (i.e., chained) to both NMOG and methane. The TOG calculator in Equation 8-4 simply adds the resulting methane emissions to the NMOG emissions.

$$\text{TOG} = \text{NMOG} + \text{Methane} \quad \text{Eq 8-4}$$

9.0 Fuel Formulation and Fuel Supply in MOVES2010

9.1 Introduction

The MOVES2010 model contains about 10,000 default fuel formulations and default market share values. The large number of fuel formulations reflects a combination of ten different fuel parameters, and the need to supply a default fuel formulation for each combination of U.S. county, month and fuel year. Each fuel formulation describes a unique set of fuel properties.

In MOVES, the fuel models (i.e., complex, predictive, sulfur, etc) are applied to each fuel formulation selected by the user. The user selects at least one fuel formulation for each county, calendar year, month and fuel type (i.e., gas or diesel) combination they wish to model. Some combinations have two or more fuel formulations which represent a blend of fuels during that time and in that area. The individual market share values represent the distribution of fuel formulations within a county, calendar year, month and fuel type combination, and must sum to unity within the combination.

9.2 Data Sources

The fuel supply and fuel formulation data in the MOVES2010 model was assembled from several sources as part of the EPA National Emission Inventory (NEI) development process. The process of assembling these data for the MOVES model consisted of a detailed analysis which is described in the references listed in Section 9.4. It consisted of a fairly complicated data review and analysis process that utilized several sources, and will not be repeated here. The following sources of fuel supply and fuel property data for MOVES are:

- EPA fuel survey data from RFG areas
- Vehicle manufacturer fuel surveys
- Other commercial fuel surveys
- Proprietary Refinery modeling results
- State supplied fuel data

The EPA fuel survey data from RFG areas is an important data source for in-use fuel property information, and market share data of specific fuels. It is an annual survey done in RFG areas. Unfortunately, it is limited to RFG areas, and often is limited to just a single county in the area. Another shortcoming is that EPA has only analyzed and incorporated surveys from the 2005 and earlier calendar years. Vehicle manufacturer and other commercial fuel surveys were also incorporated into the database, or used to confirm existing data whenever possible. The proprietary refinery modeling results were a very important source of information and allowed EPA to model areas which did not have fuel surveys. This data-source frequently had refinery, pipeline and other distribution system volume data on particular fuel formulations and individual fuel parameters such as the volume of ethanol or the concentration of sulfur in the fuel flow. The pipeline fuel flow data could be distributed according to vehicle miles traveled

(VMT) through the fuel distribution system so as to produce more complete fuel information on counties that did not have a fuel survey. State data on fuel properties and fuel supplies were also obtained and used where possible. In most cases, individual states do not have complete or detailed data on their fuel supplies.

9.3 Analysis Process Overview

An analysis process was used to assemble the MOVES fuel supply and fuel formulation tables for use in the model. For calendar years 1990, 1999, 2002 and 2005 historical fuel data were collected and processed, and used in the National Emission Inventory (NEI) process. These data were generally 'clean' and easily processed into the required format for MOVES. Analogous tables for calendar years 2000, 2001, 2003 and 2004 were generated by interpolating the primary dataset.

Calendar years 2005 and 2012 are the key years for fuel property definition. After 2012, the fuel properties and supplies become constant. The data for calendar years 2005 are from the 2005 NEI and the data (projections) for 2012 are from refinery modeling done for the RFS rulemaking. The 2012 calendar year data are projections which start with the 2005 fuels and project the 2012 fuels based on ethanol volume increases, benzene controls, MTBE phase-out and RVP waiver for ethanol blends. The impact of future fuel regulations is a major factor in these projections. Fuel data for all intervening years between 2005 and 2012 are interpolations between these two years. Local fuel regulations and local fuel data, where available, were also incorporated in the analysis for each of the counties and calendar years.

The fuel data is often only by season with winter – summer blends and one or two shoulder seasons. As a result, the data are further processed to allow it to be on a monthly basis. Frequently, in MOVES2010a, this processing consists of merely copying it into the monthly database entries. Within a given season, the fuel formulations often do not vary by month.

9.4 References

- 9.4.1 1999 NEI report that includes description of how the fuels were developed "DOCUMENTATION FOR THE ONROAD NATIONAL EMISSIONS INVENTORY (NEI) FOR BASE YEARS 1970-2002"
ftp://ftp.epa.gov/EmisInventory/finalnei99ver3/haps/documentation/onroad/nei_onroad_jan04.pdf
- 9.4.2 Updated 2002 report, "DOCUMENTATION FOR THE FINAL 2002 MOBILE NATIONAL EMISSIONS INVENTORY, VERSION 3"
ftp://ftp.epa.gov/EmisInventory/2002finalnei/documentation/mobile/2002_mobile_nei_version_3_report_09280.pdf
- 9.4.3 Updated 2005 report, "DOCUMENTATION FOR THE 2005 MOBILE NATIONAL EMISSIONS INVENTORY, VERSION 2"
ftp://ftp.epa.gov/EmisInventory/2005_nei/mobile/2005_mobile_nei_version_2_report.pdf
- 9.4.4 EPA RFG fuel survey data:
<http://www.epa.gov/otaq/regs/fuels/rfg/properf/rfgperf.htm>
- 9.4.5 RFS1 Regulatory Impact Assessment document "Draft Regulatory Impact Analysis: Changes to Renewable Fuel Standard Program"
<http://www.epa.gov/otaq/renewablefuels/420d09001.pdf>

10.0 Results

This section contains some limited emission results based on the algorithms in the Predictive, Complex and MOBILE6 Sulfur Models. These results were obtained by running the MOVES model and charting the emission results. Results are shown for the criteria pollutants and the major air toxic compounds. The results are limited in that they are shown only for areas of the MOVES model that have received substantial changes from previous versions. They are also limited because they model the base fuel and vary only one fuel parameter at a time over its range. For example, in the sulfur effects chart, fuel sulfur is varied from 4 ppm to 500 ppm and the remaining fuel parameters are kept constant at the Base Fuel level. The reader who is interested in a complete set of emission results for all combinations of fuel parameters, particularly the air toxic pollutants, should consult the primary reference documents for the Complex, Predictive and MOBILE6.2 models.

10.1 Sulfur Effects in MOVES2010a

The emission effect of fuel sulfur is shown in Figures 10-1 through 10-3 for the 2001+, 1996 and 1988 model years, respectively. The effects are 'net fuel effects' from the MOVES model. They were produced by seven separate MOVES runs using a constant fuel formulation and varying the fuel sulfur level from 4 ppm sulfur to 500 ppm sulfur. In each chart, separate curves are shown for THC, CO and NOx. The oldest model year represents the fuel effects on Tier0 vehicles, the middle model year group represents the Tier1 and LEV standards, and the 2001+ model year represents the newer vehicles. In all charts the fuel effects are normalized to 90 ppm sulfur for the 1988 and 1996 model year curve and to 30 ppm sulfur for the 2001+ model year curve. In this context, 'normalization' means the correction factor is set to one. The other fuel parameters were set at Base Fuel levels (6.9 psi RVP, 0% Ethanol volume, 26.1% aromatic content, 5.6% olefin content, 1.0% benzene content, 218F T50 and 329 F T90).

Examination of the three figures shows the strongest correlation is for NOx emissions and for the 2001+ model year group. This result is not unexpected because it is this group for which a log-log relationship between emissions and fuel sulfur was found. This relationship is strongly non-linear and produces a relative correction of about 0.15 for an ultra low 2 ppm sulfur fuel and a relative correction of about 3.0 for a 500 ppm high sulfur fuel (*actual in-use fuel sulfur levels are not expected to vary that widely*). For the HC and CO pollutants, the sensitivity to fuel sulfur is less for the 2001+ MY model year group than it is for NOx. The other model year groups mostly utilize log-linear relationships between emissions and fuel sulfur. This leads to fuel sulfur emission effects which are less sensitive to sulfur than the Tier2 group.

In the MOVES2010a model, the 2001+ model year group is the latest model year group, but is based only on data from pre-tier2 (i.e., 2003 and earlier model years) vehicles. Subsequent versions of MOVES (to be released at a later date) will utilize these curves for the 2001 through 2003 model years, but will apply new curves for 2004 and later model years based on a new set of vehicle fuel sulfur testing and EPAAct testing. Preliminary results from the analysis of the new data suggests a much stronger

relationship at low sulfur levels between fuel sulfur and HC and NOx emissions than is used in MOVES2010a.

No air toxic charts are shown because the air toxic / VOC ratio is not a function of fuel sulfur level in the Complex model.

Figure 10-1 Relative Fuel Sulfur Effect on 2008 Model Year Gasoline Vehicles in MOVES

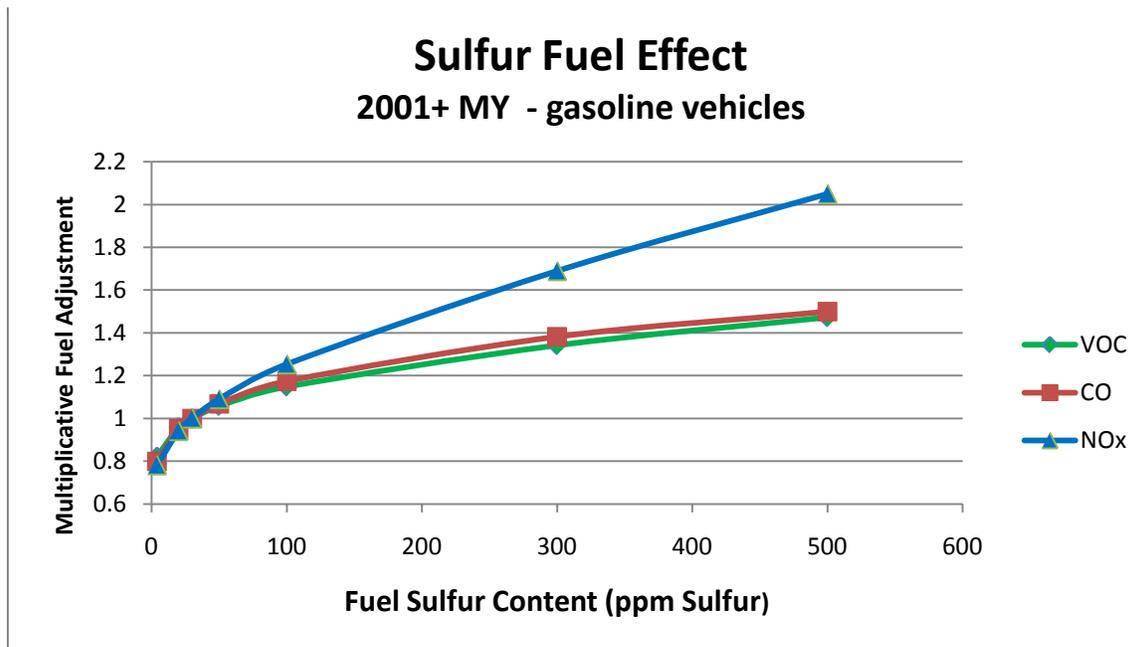


Figure 10-2 Relative Fuel Sulfur Effect on 1996 Model Year Gasoline Vehicles in MOVES

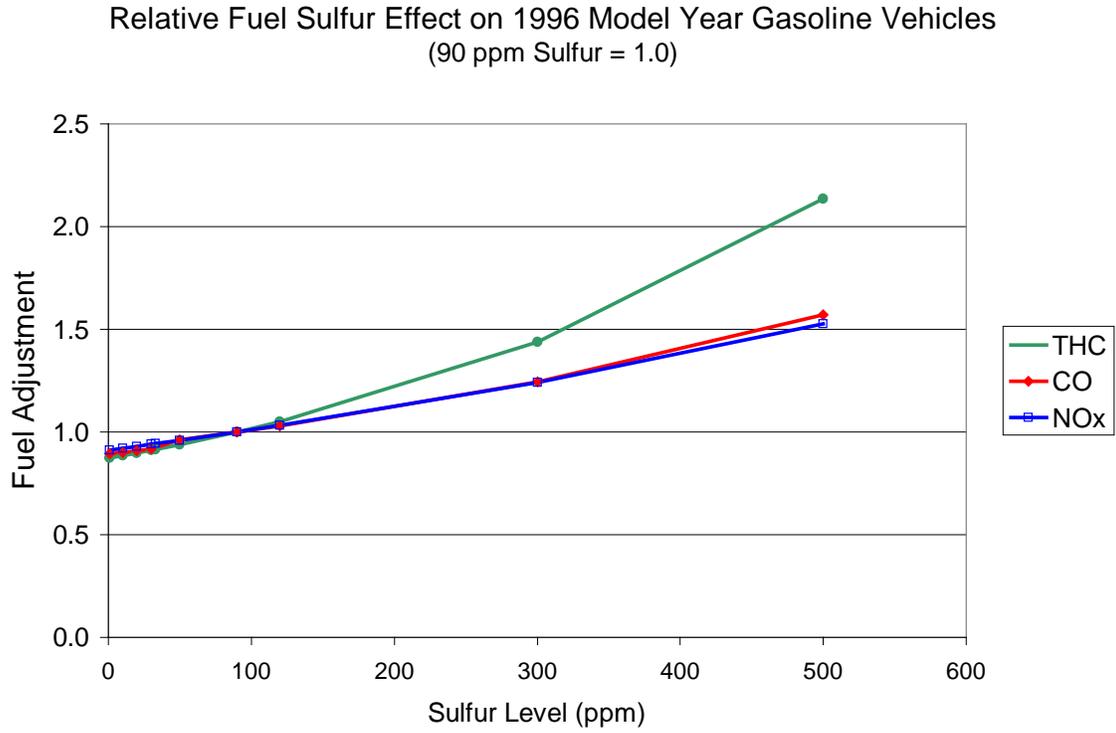
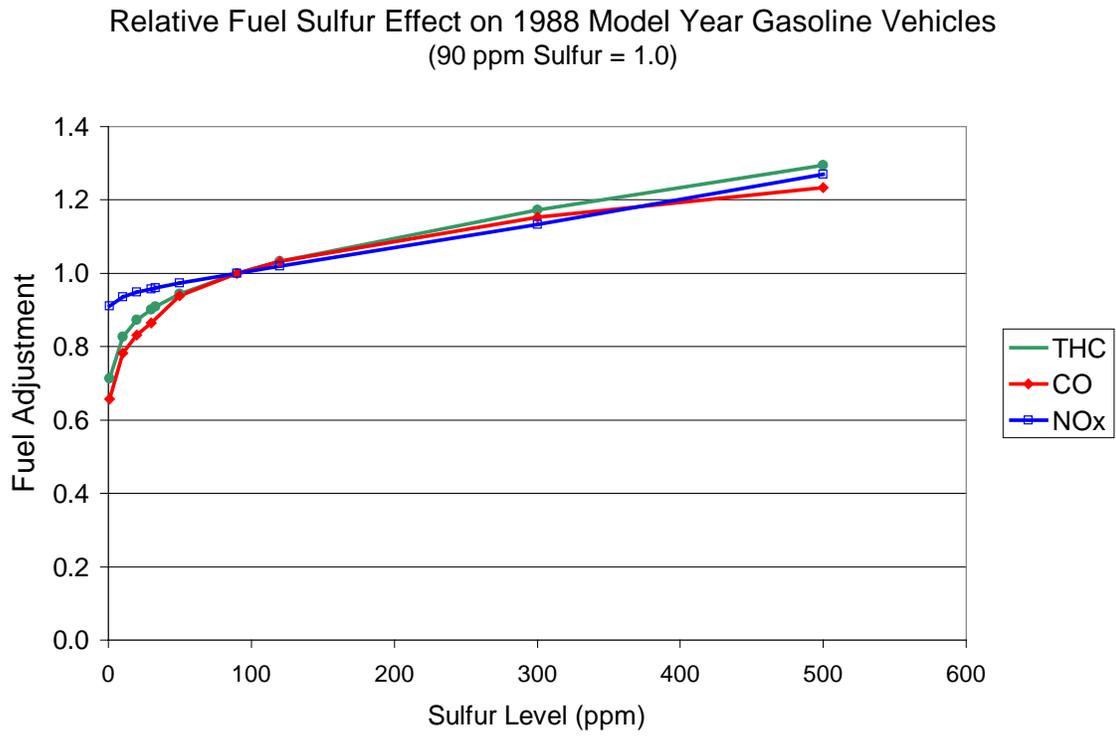


Figure 10-3 Relative Fuel Sulfur Effect on 1988 Model Year Gasoline Vehicles in MOVES



10.2 Fuel Ethanol Adjustment Factors in MOVES2010

The emission effects of fuel ethanol are shown in Figure 10-4 for model year 2003. Charts for other model years are not shown, because the results are similar for the pre-1994 model years (they differ only slightly for CO) and are identical for the 1995-through-2002 model years. There are currently no ethanol fuel effects for 2004-and-later model years in MOVES2010a (only sulfur fuel effects). Other fuel oxygenate types such as MTBE or ETBE produce the same relative results when the oxygenate volumes are identical. The other fuel parameters were set at Base Fuel levels (6.9 psi RVP, 30 ppm sulfur level, 26.1% aromatic content, 5.6% olefin content, 1.0% benzene content, 218F T50 and 329 F T90).

The effects shown in the chart are 'net fuel effects' from the MOVES model. They were produced with three separate MOVES runs using a constant fuel formulation and varying the fuel ethanol level from 0 percent to 15 percent by volume. In each chart, separate curves are shown for THC, CO and NOx. In all curves the fuel effects are normalized to 10 percent volume ethanol. In this context, 'normalization' means the correction factor is set to unity with the ethanol volume is 10 percent.

Overall, the results are as expected with only small changes in THC emissions, moderate reductions in CO emissions, and NOx emission increases from the use of ethanol. For HC and NOx, there is about a five percent increase from zero ethanol to 10 percent ethanol. Carbon monoxide emissions show approximately a 15 decrease from zero ethanol to 10 percent ethanol. This is likely due to the extra oxygen introduced by ethanol into the combustion and exhaust process that oxidizes the carbon monoxide to carbon dioxide. In MOVES2010a, there are no fuel effects on particulate matter (PM) emissions.

Figure 10-4 Relative Fuel Ethanol Effect on Pre-2004 Model Year Gasoline Vehicles in MOVES

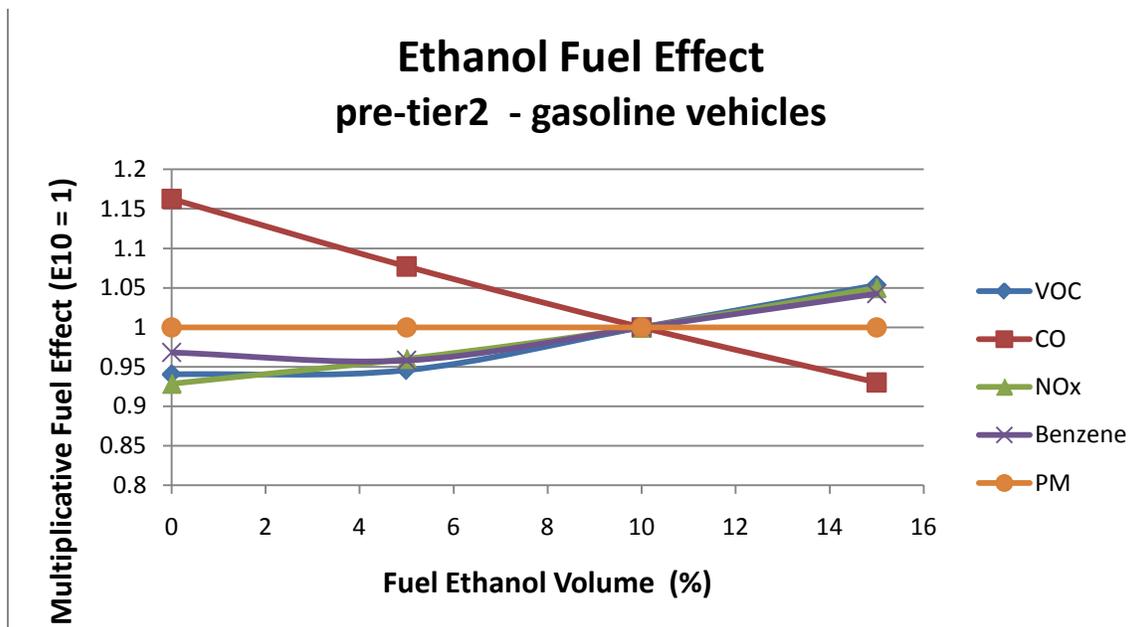


Figure 10-5 Relative Fuel Ethanol Effect on Pre-2004 Model Year Gasoline Vehicles in MOVES

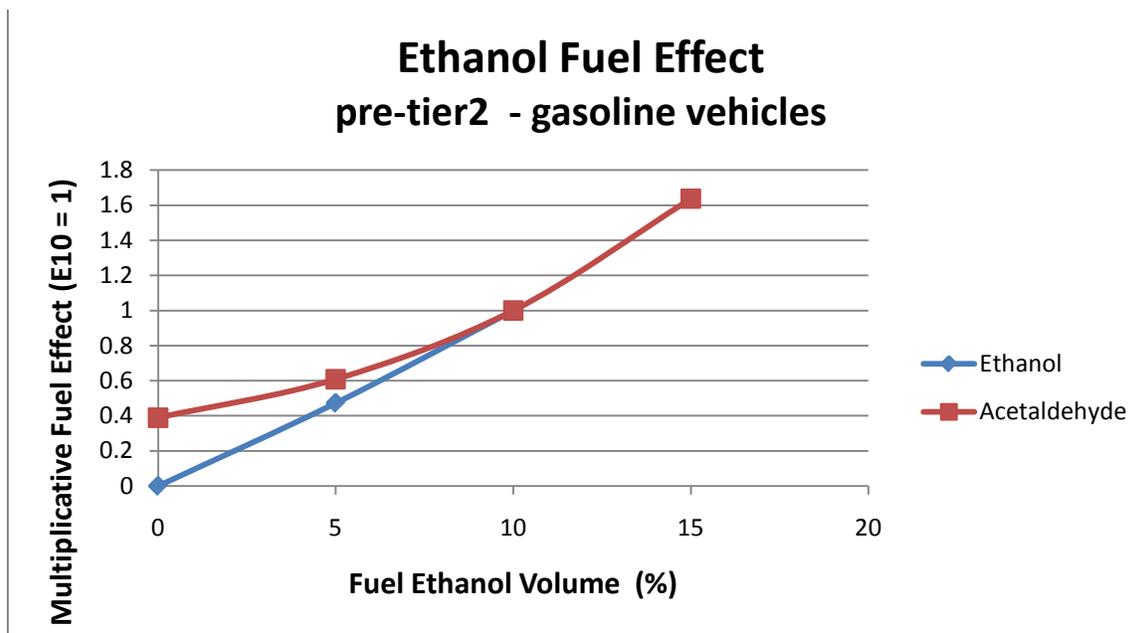


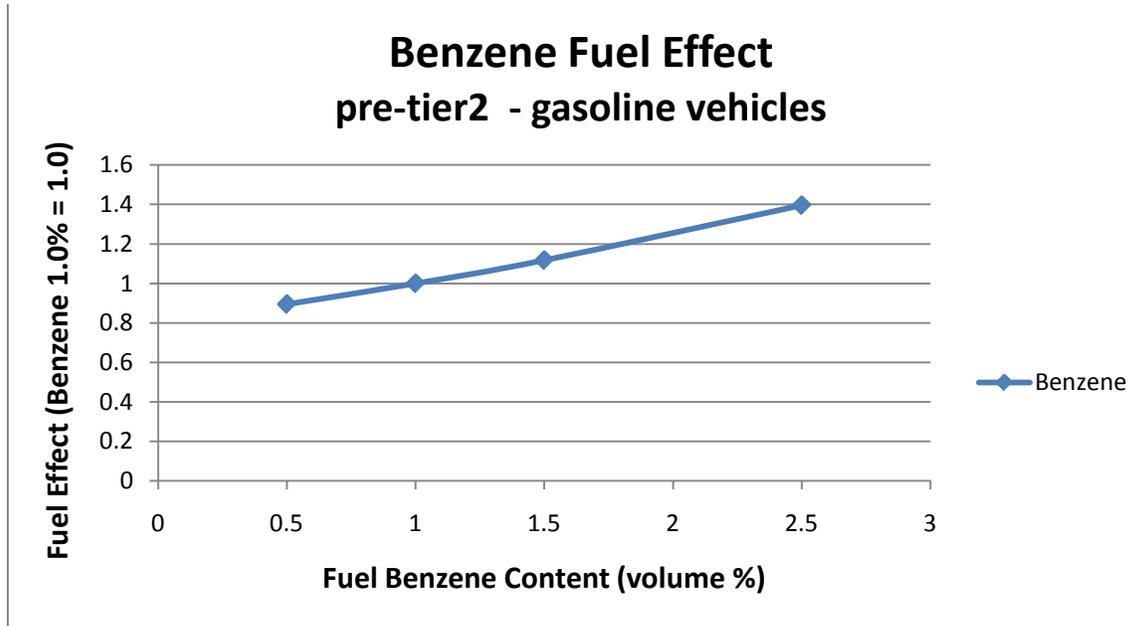
Figure 10-5 shows the relationship between fuel ethanol and exhaust ethanol and acetaldehyde emissions. These are shown on a separate figure because the fuel effects range from zero to almost a factor of two for these two air toxic pollutants. Both these curves show a strong and predictable response to fuel ethanol from 0 to 10 percent ethanol.

Figures 10-4 and 10-5 show a maximum value of 15 percent. However, users should not attempt to model higher ethanol inputs such as 15 percent ethanol (E15) or 85 percent ethanol (E85) with MOVES2010a. For ethanol values greater than 10 percent, the relationships in MOVES2010a are pure extrapolation. Future versions of MOVES will show updated relationships based on recent vehicle testing, rather than mathematical extrapolations.

10.3 Benzene Adjustment Factors in MOVES2010a

The emission effects of fuel benzene are shown in Figure 10-6 for model year 2003. Charts for other model years are not shown, because the results are similar. Fuel benzene levels affect only exhaust and evaporative (not shown) benzene emissions. Figure 10-6 shows the relative effect of fuel benzene on benzene exhaust emissions with a relative effect of unity assigned to a fuel benzene level of one percent. The effect is positive and generally linear over the range of fuel benzene in use.

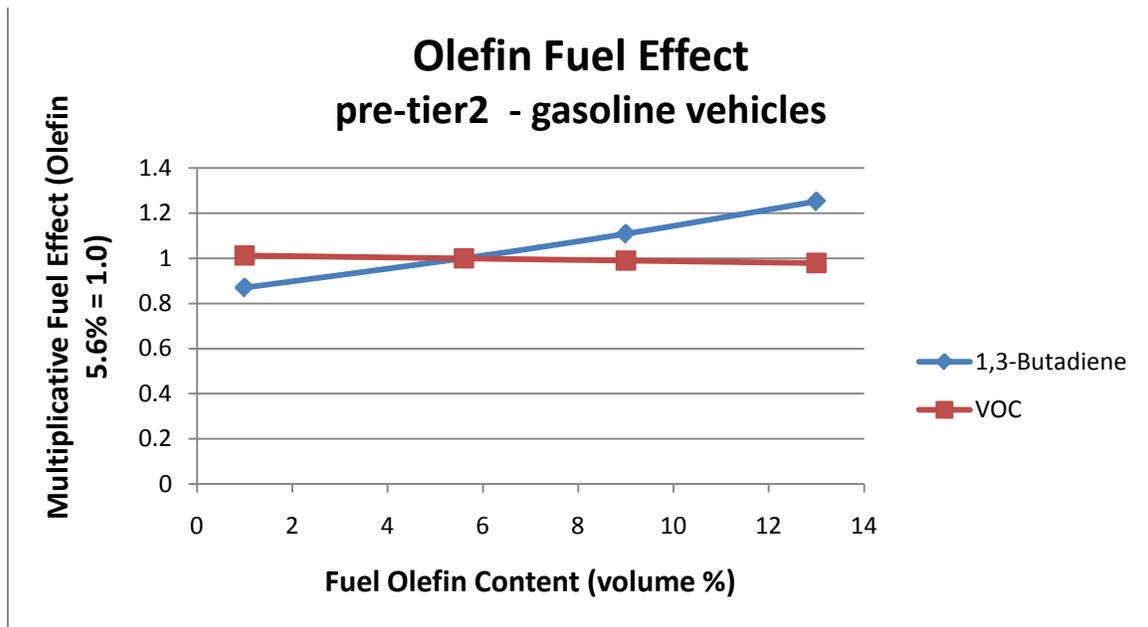
Figure 10-6 Relative Fuel Benzene Effect on Pre-2004 Model Year Gasoline Vehicles in MOVES



10.4 Olefin Adjustment Factors in MOVES2010a

Figure 10-7 shows the relative effect on pre-2004 model year gasoline vehicles to fuel olefin levels. The relative effect of unity is assigned to a fuel olefin level of 5.6% because that is the olefin level of the MOVES2010a reference fuel. Only pollutants VOC and 1,3-butadiene are affected by fuel olefin levels. The VOC response is slightly negative, but the 1,3-butadiene response is positive and quite significant over the range of olefin levels in use. The other fuel parameters were set at Base Fuel levels (6.9 psi RVP, 30 ppm sulfur level, 0% Ethanol volume, 26.1% aromatic content, 1.0% benzene content, 218F T50 and 329 F T90).

Figure 10-7 Relative Fuel Olefin Effect on Pre-2004 Model Year Gasoline Vehicles in MOVES

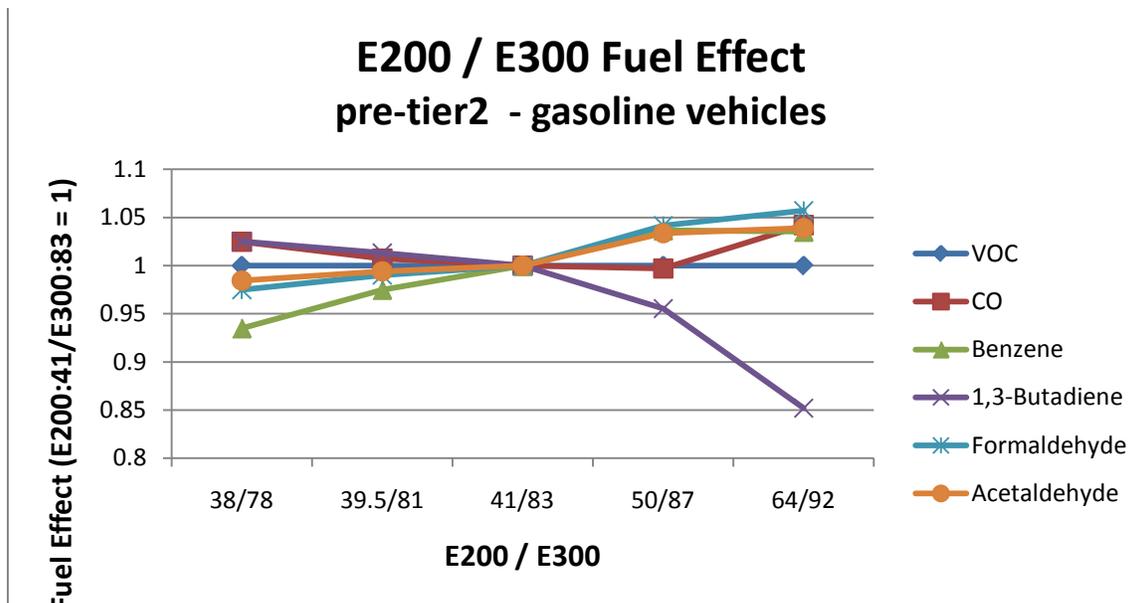


10.5 E200 / E300 Adjustment Factors in MOVES2010a

Figure 10-8 shows the relative effect on pre-2004 model year gasoline vehicles to fuel E200 and E300 levels. The relative effect of unity is assigned to a fuel e200 level of 41% and a fuel E300 level of 83% (T50 and T90 are 218F and 329F, respectively) because those are the levels in the MOVES2010a reference fuel. The parameters E200 and E300 are measures of gasoline volatility, and are shown as a pair in Figure 10-8. In this example, both move as a pair either up or down from the 41%/83% reference. In-use, this relationship between E200 and E300 does not always occur. Also, some of the values of E200 and E300 cannot occur in conjunction with the Base Fuel parameters. The E200 / E300 domain in Figure 10-8 is the entire range of values in the MOVES fuel database, and the two points at the end of the curves are extreme values. The other fuel parameters were set at Base Fuel levels (6.9 psi RVP, 30 ppm sulfur level, 0% Ethanol volume, 26.1% aromatic content, 5.6% olefin content and 1.0% benzene content).

The pollutants VOC and CO are both affected by E200 / E300 and so are most of the air toxic pollutants. Most of the pollutants increase as E200 / E300 become larger (i.e., the fuel contains a larger fraction of heavier constituents). The exception is 1,3-butadiene which shows a negative relationship with E200 / E300.

Figure 10-8 Relative Fuel E200 / E300 Effect on Pre-2004 Model Year Gasoline Vehicles in MOVES



Appendix A Peer Review

A preliminary draft version of this document was peer reviewed by Professor Tom Durbin, Ph.D Research Engineer at the University of California, CE-CERT, Riverside, CA. Many of his comments were addressed in this final version; some sections of draft report were removed altogether from the final report. Professor Durbin made seventeen distinct comments. These are paraphrased in italics, and addressed below. The full text of Professor Durbin's comments is available in a separate document.

1. *The document should have a formal reference section.*

We have added footnotes to the document and plan a references page. Web links are inserted throughout the document for important reference documents.

2. *Abbreviations should be better defined in the document.*

We agree and have addressed this comment.

3. *It would be interesting if the document could tie in the written text with the Appendices with the code.*

Between the draft that Prof. Durbin reviewed and the release of MOVES2010, much of the work that was done outside the model was incorporated in the MOVES code and the need for the fuel binner was eliminated. For more detail on the MOVES code itself, see the MOVES "Software Design Reference Manual" and the "Programmer's Guide to MOVES."

4. *Since the values for the fuel formulation table are described in greater detail later in the document, it might be useful to indicate that these variables will be discussed in the greater detail in the document.*

Section 9.0 of the document has been added to provide an overview of the fuel formulation and fuel supply development process. It describes the process of developing these critical data tables and provides a list of references to the primary documents.

5. *There is not a good logical development of the thoughts in Section 2.*

The draft version reviewed by Professor Durbin has been thoroughly revised, and we hope it contains a clearer description of the Complex model structure.

6. *The concept of using the 30 ppm fuel for the 2001 and later model year vehicles and using the 90 ppm fuel for all 2000 and earlier model years is not very clear.*

Unfortunately, the fuel properties of the vehicle dataset used to develop the basic emission factors were not measured with any real precision. The value of 30 ppm sulfur was chosen because is it the standard reference case for most EPA fuel models, and was the assumed in-use fuel standard during the latter period of testing Arizona. The value of

90 ppm sulfur was a typical value during the beginning of the Arizona test period. The value of 90 ppm comes with considerable uncertainty.

7. *A slight expansion of the GPA regions would be useful.*

This section has been expanded in the final version.

8. *There should be some discussion as to what oxygenate factors are used for different cases with ethanol, MTBE, and TAME. It might be interesting to include some statistics in the document about what percent of fuels contained these various oxygenates. That would provide the reader a good context for the relative importance of as to how fuel formulations have changed over time.*

We did not provide the statistics, but they could be developed with effort from the MOVES Fuel Supply and Fuel Formulation tables. In general, the calendar year 2005 and earlier generally contain modest amounts of MTBE as the primary oxygenate. After calendar year 2006, MTBE declines dramatically because of ground water contamination concerns and is replaced almost exclusively by Ethanol. TAME and ETBE were never major oxygenate sources and rarely achieve more than a five percent market share. In current years (i.e., 2010+) they are all but gone from the fuel mix.

9. *This comment address fuel supplies and the fact that MOVES does not contain default fuel supplies past calendar years 2012.*

This topic has been removed in the final draft because it pertains to the detailed fuel supply data and statistics which are now outside the scope of the document. However, the default MOVES only contains fuel supply information through 2012. As this date approaches, this limitation will have to be addressed. For current State Implementation Plan (SIP) work, users are expected to enter their own fuel supply information for ALL years. Once the user supplied data is entered, the model correctly performs all of the fuel calculations.

10. *A mostly editorial comment regarding clarity on E10, E85 and NMIM.*

The topics of E85 and NMIM have been completely removed from the document.

11. *A comment regarding at 2022 fuel supply database.*

This topic has been completely removed from the document.

12. *An editorial comment on the Predictive model.*

The Predictive model is now built directly into MOVES and is fully documented in Section 4.0

13. *A comment on High emitters with the question “What information was used to come up with the 20% estimate for high emitters”.*

This assumption has been changed. The new MOVES algorithm now uses the High emitter fraction from MOBILE6.2 that is a function of age (0 through 30). The calculation of High emitters is fully document in the MOBILE6.2 documentation.

14. *The assumption that NOx and THC emissions for 1994 and newer vehicles are no longer sensitive to the effects of fuel parameters outside of the sulfur is a very large simplification of the situation. Of the fuel parameters, the addition of oxygenates / ethanol is one area that would seemingly be fairly critical given that the levels of ethanol in gasoline will be increasing. He subsequently cites studies to boost his argument.*

We agree that the 1994 and later assumption was too much of a simplification and changed the assumption to 2004 and later model years. The 2003 and earlier years are now fully affected by all of the fuel parameters as appropriate for the pollutant.

15. *The Fuel Binner code is not in Appendix A.*

MOVES no longer requires fuel binning, so this code is no longer relevant.

16. *What is the basis for the EPA belief that Tier2 vehicles are less sensitive to fuel properties other than sulfur?*

At the time of this document development, the EPAAct vehicle – fuel study had not been completed and its results could not be incorporated into the model. Based on very limited knowledge of those vehicles, we made the assumption that 2004 and later model years (i.e., Tier2) vehicles are only sensitive to fuel sulfur in MOVES2010a.

Since the release of MOVES2010a, the EPAAct study and the statistical analysis of the results have been completed, and these show that Tier2 vehicles are quite sensitive to an entire range of fuel properties depending on pollutant. Subsequent versions of MOVES will incorporate these new findings.

17. *Professor Durbin includes a set of grammatical and editorial comments.*

The document has been restructured and revised to address these comments.