< Chapter in: Report: *Modeling Effects of Fuel Properties in the Motor Vehicle Emissions Simulator (MOVES2014): DRAFT Report*.

Gasoline Fuel Effects for Vehicles certified to Tier-2 Standards

Contents

1 Introduction

An important function of mobile source air pollution inventory models, including MOBILE6 and MOVES, is to account for the effects of different fuel properties on exhaust emissions. For this purpose, MOBILE6 relied on previously existing fuel effect models, known as the "EPA Predictive Model" and the "Complex Model". These models were developed using data collected on 1990s-technology vehicles meeting the Tier 0 and Tier 1 emission standards, levels an order of magnitude higher than those for currently manufactured vehicles compliant with Federal Tier-2 or equivalent LEV-II standards. While these models are still in use in MOVES to estimate fuel effects for vehicles manufactured prior to model year 2001--for example, equations from the Predictive Model are used to calculate fuel effects for total hydrocarbons and oxides of nitrogen, and equations from the Complex Model are used to estimate fuel effects for toxic compounds, including carbon monoxide and air toxics, such as benzene and the aldehydes[1]--their applicability to vehicles employing more recent engine and emission control technologies has been questioned. Since the initiation of the MOVES project, it has become clear that an updated fuel-effects model representing Tier-2 certified vehicles would be needed. In addition, Congress provided for the development of such a model in the 2005 Energy Policy Act (EPAct).

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

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

Initiated in March 2009, the Phase 3 program involved measurement of exhaust emissions from fifteen high-sales-volume Tier-2 certified vehicles (model year 2008), using twenty-seven test fuels spanning wide ranges of five fuel properties (ethanol, aromatics, vapor pressure, and two distillation parameters: T50 and T90). The properties of the test fuels were not assigned to represent in-use fuels, but rather to allow development of statistical models that would enable estimation of relative differences in emissions across the ranges of fuel properties expected in the U.S. fuel pool. A fuel matrix was designed for Phase 3 to span the ranges of the five selected properties seen in commercially available fuels.

An initial sample of 19 test vehicles was chosen with the intent of representing the latest-technology light-duty vehicles being sold at the time the program was launched (model year 2008). The 19 vehicles represented a high fraction of vehicle sales at the time. The sample was to conform on average to Tier-2 Bin-5 exhaust levels and employ a variety of emission control

technologies, to be achieved by including a range of vehicle sizes and manufacturers. Due to budget constraints, the sample was reduced from 19 to 15 vehicles for the Phase-3 program.

The LA92 test cycle was used with emissions measured over three phases analogous to those in the Federal Test Procedure (FTP), at an ambient temperature of 75°F. In MOVES, the EPAct results are applied at temperatures higher and lower than this level, under an assumption that effects for fuels and temperature are independent and multiplicative.

Emissions measured include carbon dioxide (CO_2), carbon monoxide (CO), total hydrocarbons (THC), methane (CH_4), oxides of nitrogen (NO_x), and particulate matter ($PM_{2.5}$). In addition, hydrocarbons were speciated for subsets of vehicles and fuels, allowing calculation of derived parameters such as non-methane organic gases (NMOG) and non-methane hydrocarbons (NMHC). Speciation also allowed independent analyses of selected toxics including acetaldehyde, formaldehyde, acrolein, benzene and 1,3-butadiene.

Phase 3 data collection was completed in June 2010. Dataset construction and analysis was conducted between January 2010 and November 2012. This process involved ongoing collaboration among EPA staff, DOE staff and contractors, and CRC representatives. Following the completion of data collection, construction of the dataset involved intensive evaluation and quality assurance. The analysis involved several iterations between analysis and additional physical and chemical review of the data. Successive rounds of statistical modeling were applied to the data, to achieve several goals, including identification of potential candidate models, identification and review of outlying observations, identification and review of subsets of data from influential vehicles, and identification of models including subsets of terms that best explain the results obtained.

The EPAct exhaust research program and analysis are extensively documented in the "EPAct Test Program Report" [2] and "EPAct Analysis Report."[3]

This chapter describes how the statistical models developed during the EPAct study are applied in the MOVES model (MOVES2014).

2   Scope and Implementation

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

Fuels: The adjustments apply to gasoline (fueltypeID = 1). The adjustments described in this document are applied to gasoline blends containing 0-20% ethanol.

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

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

SourceType: The adjustments apply to all sourceTypes.

Emission Processes: Adjustments are developed and applied separately to running exhaust (processID = 1) and start exhaust emissions (processID = 2). Fuel adjustments for evaporative emissions are described (add reference to evap report)

Pollutants: The pollutants covered include those listed in Table 1.

Table 1. Pollutants Modified by Fuel Adjustments

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

Database Table: MOVES2014 allows a very flexible input data format for incorporating and applying coefficients within a wide variety of mathematical forms. These "fuel-effect ratio expressions" can include up to 32,000 characters and are stored in a database table dedicated to this purpose (GeneralFuelRatioExpression). See Section 4 (page 10) for a more detailed description of the table.

2.1   Standardizing Fuel Properties

In applying the EPAct models to estimate emissions effects for a given fuel, it is necessary to first "center" and "scale" the properties for the fuel, a process also known as "standardization." This process simply involves first "centering" the measured fuel properties by subtracting the given value from the sample mean, and then "scaling" by then dividing the centered values by their respective standard deviations (with the means and standard deviations calculated from the

fuel set used in the study), as shown in Equation 1. The result is a "Z score," representing a "standard normal distribution" with a mean of 0.0 and a standard deviation of 1.0.

$$Z_i = \frac{x_i - \overline{x}}{s}$$ **Equation 1**

For the linear effects in the model, standardization is performed using the values of each fuel property, each in their respective scales (vol. %, psi, °F.). Using aromatics as an example, the standardization of the linear term is shown in Equation 2.

$$Z_{arom} = \frac{x_{arom} - \overline{x}_{arom}}{s_{arom}}$$ **Equation 2**

For second-order terms, however, the process is not performed on the values of the fuel properties themselves. Rather, quadratic and interaction terms are constructed from the Z scores for the linear terms, and the process is repeated. This step is taken to neutralize correlations between second-order terms and the linear terms from which they were constructed. Using the quadratic term for ethanol as an example (etOH×etOH), the standardized value, denoted by $ZZ_{etOH \times etOH}$, is calculated as shown in Equation 3, where $m_{Z_{etOH}Z_{etOH}}$ and $s_{Z_{etOH}Z_{etOH}}$ are the mean and standard deviation of the quadratic term constructed from the Z score for the linear effect.

$$ZZ_{etOH \times etOH} = \frac{Z_{etOH}Z_{etOH} - m_{Z_{etOH}Z_{etOH}}}{s_{Z_{etOH}Z_{etOH}}}$$ **Equation 3**

Standardized terms for interaction effects are constructed similarly. For example, Equation 4 shows the standardization of an interaction term between ethanol and aromatics.

$$ZZ_{etOH \times eArom} = \frac{Z_{etOH}Z_{Arom} - m_{Z_{etOH}Z_{Arom}}}{s_{Z_{etOH}Z_{Arom}}}$$ **Equation 4**

Means and standard deviations for relevant model terms designs are shown in Table 2.

Table 2. Means and Standard deviations for Fuel Properties, based on Fuel Matrix in the EPAct Phase-3 Project.[1]

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

3 Fuel Effect Adjustments

In MOVES, emissions of the pollutants THC, CO, NO_x and PM are calculated starting with "base emission rates" (meanBaseRate, meanBaseRateIM) stored in the database table, emissionRateByAge[4]. The base rates are assumed to represent emissions on a "base fuel" which are multiplied by an adjustment to represent emissions on a selected in-use fuel. Different fuel adjustments have been developed to represent selected pollutants and emission processes. Adjustments also vary depending on vehicle type and model year. A general discussion of the development and application of fuel effects used in MOVES2010 is provided in a separate technical report.[5] This document describes the application of the EPAct study results to derive fuel adjustments for the subsets of vehicles and model years described above.

The models generated using EPAct results allow estimation of emissions effects related to five fuel properties: ethanol content (%), aromatics content (%), RVP (psi), T50 (°F) and T90 (°F), as well as selected interaction terms among these five parameters. The statistical models generated from the EPAct exhaust data follow the general structure shown in Equation 5 below. In this example equation, β denotes a model coefficient, Z_{etOH} denotes a "standardized" fuel term for this property, and $Z_{etOH \times Arom}$ denotes a "standardized" etOH×Arom interaction term.[1] For

---

[1] Note that these coefficients apply to fuel properties that have been "standardized," i.e., centered on their means and scaled by their standard deviations, based on the fuel-property matrix used to develop the models. To properly apply the models, this process must be applied for the specific fuels under consideration. For more information on this technique, please see the EPAct analysis report.

simplicity, the terms for ethanol and the etOH×Arom interaction have been shown; linear and interaction terms for the remaining three properties are not shown in this example. Finally, the term s_ε^2 represents the residual error or "mean square error" for the model. Note that the subsets of the potential terms vary by emission and process, depending on the results of the statistical model fitting.

Two sets of exhaust fuel effect coefficients were employed for each pollutant; one set representing start emissions and a second set representing hot-running emissions. In some cases fuel effects estimated for these two processes differed substantially, as the effects of fuel properties on start emissions are dominated by changes in combustion and catalyst warm-up, while the impact of running emissions is dictated by catalyst efficiency when fully operational.

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

$$\text{Emissions (g/mi)} = e^{\mathbf{X\beta}}$$
$$= \exp\begin{pmatrix} \beta_0 + \beta_{etOH}Z_{etOH} + [\textit{other linear terms}] + \beta_{etOH \times Arom}Z_{etOH \times Arom} + \\ [\textit{other 2nd-order terms}] + 0.5s_\varepsilon^2 \end{pmatrix} \qquad \textbf{Equation 5}$$

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

Table 3 shows the coefficients used in Equation 6 for four individual pollutants, including total hydrocarbons (THC) and the criteria pollutants CO, NO$_x$, and PM. The application of these models has been integrated into MOVES2014. For implementation in MOVES, Equation 6 is input directly into the GeneralFuelRatioExpression table.

The table presents two sets of coefficients for each pollutant, representing the effects of the fuel properties on start and running exhaust emissions, respectively.[2] The coefficients can be understood as the change in the natural logarithm of emissions (e.g., ΔlnCO) associated with a change in the fuel property of 1.0 standard deviation. Because these coefficients apply to "standardized" fuel properties, as mentioned above, the magnitude and signs of the terms are comparable, giving a sense of the influence of each term in the estimation of that pollutant relative to the others. For example, for PM start emissions, changes in aromatics and T90 are very influential, and are positively related with PM emissions (e.g., when aromatics increase, PM increases). For THC start emissions, on the other hand, the negative sign of the coefficient

---

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

indicates that the relationship is inverse, i.e., increases in RVP are associated with decreases in THC.

Table 3. Standardized Coefficients for Models representing Regulated Gaseous Emissions and Particulates, from the EPAct Program.

Model Term	THC		CO		NO$_x$		PM	
	Start	*Running*	*Start*	*Running*	*Start*	*Running*	*Start*	*Running*
Intercept	-0.8664	-4.6533	1.3466	-1.3893	-2.8594	-4.5692	0.6559	-1.3107
etOH	0.0548	0.0327	-0.1049		0.06750	0.06299	0.1582	0.1126
aromatics	0.0676	-0.0195	-0.01242	0.0913	0.1339	0.04407	0.3833	0.1662
RVP	-0.0445	-0.0355	-0.00762	0.0299				
T50	0.1288	0.0501	-0.03273	0.0261	0.04783		0.0550	
T90	0.0183	0.0514	-0.1571	0.0440			0.2923	0.1072
etOH×etOH	0.0436		0.07304					
T50×T50	0.0736	0.0337	0.05358				0.0935	
etOH×Arom	0.0179		0.02086		-0.02369			
etOH×RVP			0.01596					
etOH×T50	0.0445		0.1064					
etOH×T90	0.0214							
Variance (s^2_ε)	0.2012	0.9057	0.4641	2.0443	0.7383	0.6556	1.4610	1.9164

4 The Database Table "GeneralFuelRatioExpression"

As mentioned, the models shown in Equation 5 and Equation 6, applying coefficients as shown in Table 3, are stored in the database table "GeneralFuelRatioExpression." A description of this table is shown in Table 4.

Table 4. Description of the Database Table "GeneralFuelRatioExpression."

Field	Description	Values
fuelTypeID	Identifies fuel types as broad classes, i.e., "gasoline," "diesel," etc.	1 = gasoline 2 = diesel, Etc.
polProcessID	Identifies combinations of pollutant and process.	e.g., 301 = hot-running NOx, etc.
minModelYearID	The earliest model year to which a specific value of fuelEffectRatioExpression is applied.	e.g., 2001
maxModelYearID	The latest model year to which a specific value of fuelEffectRatioExpression is applied.	e.g., 2050
minAgeID	The minimum vehicle age at which the value of fuelEffectRatioExpression is applied.	e.g., 0 years
maxAgeID	The maximum vehicle age at which the value of fuelEffectRatioExpression is applied.	e.g., 30 years
sourceTypeID	Identifies vehicles by functional type. See table "sourceUseType."	11= motorcycle 21= passenger car 31=passenger truck 32=light commercial truck, etc.
fuelEffectRatioExpression	A mathematical expression containing up to 32,000 characters.	

4.1 Example

We show an example of an application of a fuel adjustment for cold-start NOx applied in conjunction with the adjustment for fuel sulfur. Note that the adjustment for sulfur is calculated independently of that for the other properties: ethanol, aromatics, vapor pressure, T50 and T90. The calculation of adjustments for sulfur content is described in Chapter X.X in this document. The entire expression is show below in Table 5. Due to its length, the whole is divided into terms and segments and described in Table 6.

Table 5. Example Value for Field "fuelEffectRatioExpression" in Database Table "GeneralFuelRatioExpression" (NOTE: this example calculates an adjustment for cold-start NOx, accounting for the fuel properties: ethanol, aromatics, vapor pressure, T50, T90 and sulfur).

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

Table 6. Expression stored in the Field "fuelEffectRatioExpression" in the Table "GeneralFuelRatioExpression."

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

5   References

[1] U.S. EPA. MOVES2010 Fuel Adjustment and Air Toxic Emission Calculation Algorithm – Development and Results.

[2] U.S. EPA. EPAct/V2/E-89: *Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles certified to Tier-2 Standards: Final Report on Program Design and Data Collection*. EPA-420-R-13-004. Assessment and Standards Division, Office of Transportation and Air Quality, Ann Arbor, MI; National Renewable Energy Laboratory, Golden, CO; Coordinating Research Council, Alpharetta, GA. April, 2013.

[3] U.S. EPA. *Assessing the Effect of Five Gasoline Properties on Exhaust Emissions from Light-Duty Vehicles certified to Tier-2 Standards: Analysis of Data from EPAct Phase 3 (EPAct/V2/E-89). Final Report*. EPA-420-R-13-002. Assessment and Standards Division, Office of Transportation and Air Quality, Ann Arbor, MI. April, 2013.

[4] U.S. EPA. 2011. *Development of Emission Rates for Light-Duty Vehicles in the Motor Vehicle Emissions Simulator (MOVES2010)*. EPA-420-R-11-011. Assessment and Standards Division, Office of Transportation and Air Quality, Ann Arbor, MI. August 2011.

[5] U.S. EPA, 2011. MOVES2010 Fuel Adjustment and Air Toxic Emission Calculation Algorithm – Development and Results (EPA-420-R-11-009)
http://www.epa.gov/otaq/models/moves/documents/420r11009.pdf