CRC Report No. A-73-1

Development of Inventory and Speciation Inputs for Ethanol Blends

Final Report

May 2012

COORDINATING RESEARCH COUNCIL, INC.
3650 MANSELL ROAD·SUITE 140·ALPHARETTA, GA 30022

The Coordinating Research Council, Inc. (CRC) is a non-profit corporation supported by the petroleum and automotive equipment industries. CRC operates through research committees made up of technical experts from industry and government who voluntarily participate. The four main areas of research within CRC are: air pollution (atmospheric and engineering studies); aviation fuels, lubricants, and equipment performance; heavy-duty vehicle fuels, lubricants, and equipment performance (e.g., diesel trucks); and light-duty vehicle fuels, lubricants, and equipment performance (e.g., passenger cars). CRC's function is to provide the mechanism for joint research conducted by the two industries that will help in determining an optimum combination of petroleum products and mobility equipment. CRC's work is limited to research that is mutually beneficial to the two industries involved. Final reports and data are made available to the public.

sierra research

Report No. SR2012-05-01

Development of Inventory and Speciation Inputs for Ethanol Blends

prepared for:

Coordinating Research Council, Inc.
3650 Mansell Road, Suite 140
Alpharetta, GA 30022

May 2012

prepared by:

Sierra Research, Inc.
1801 J Street
Sacramento, California 95811
(916) 444-6666

Report No. SR2012-05-01

Development of Inventory and Speciation Inputs for Ethanol Blends

prepared for:

Coordinating Research Council

May 2012

Jeremy G. Heiken
James M. Lyons

Sierra Research, Inc.
1801 J Street
Sacramento, CA 95811
(916) 444-6666

Development of Inventory and Speciation Inputs for Ethanol Blends

Table of Contents

List of Tables

Table Page

1. EXECUTIVE SUMMARY

In order to assess the potential air quality impacts of ethanol use in gasoline, the Coordinating Research Council (CRC) initiated two related projects: A-73-1 and A-73-2, with the former focused on the development of emission inventory and speciation data needed to drive a photochemical modeling study assessing those impacts, and the latter focused on the photochemical modeling assessment itself. This report documents the A-73-1 project in which detailed inventory and speciation methods and inputs were developed for the air quality assessment for specific ethanol-blend scenarios.

The purpose of this study was to use the best data available to create the requisite emission inventory processing inputs for the following four scenarios:

1. 2005 base year inventory and use of historical fuels;

2. 2020 future year inventory and nationwide 10 percent by volume ethanol blend usage (i.e., E10);

3. 2020 future year inventory and nationwide 15 percent by volume ethanol blend usage (i.e., E15); and

4. 2020 future year inventory and nationwide 20 percent by volume ethanol blend usage (i.e., E20).

Emission inventory and speciation inputs were developed to reflect the use of distinct ethanol blends (E0 through E20) defined by these scenarios.[1] The inventory modeling domain was the lower 48 states of the U.S., with inventories defined at the county level. The results of this evaluation were detailed inventory and speciation datasets that allowed for an inventory assessment of any part of the modeling domain or the domain as a whole.

Specifically, the resulting data from this study are in the two forms described below.

1. *Emission inventory adjustment factors* were developed as multiplicative inventory corrections as described in Section 3 of this report. These factors incorporate new fuel correction methods and are defined to convert a preexisting on-road inventory over to the conditions of each scenario.

[1] E0 is used herein as an abbreviation for ethanol-free gasoline.

2. *HC speciation inputs* were developed representing each scenario as described in Section 4. These data convert the aggregate HC inventory results into the class of species defined by the Carbon Bond mechanism (Version 5) used to support photochemical modeling.

The methods and results of this project were based on and designed to work with the emission modeling tools described below.

1. MOVES2010a – The on-road inventory methods for modeling ethanol blends up to 20 percent by volume were specifically defined to work with the current version of EPA's MOVES model.[2] Updated fuel correction methods and scenario-specific gasoline assumptions were incorporated into inventory adjustment factors, to be applied as a post-model adjustment (such that no modifications were made to the model itself). MOVES2010a is capable of modeling ethanol blends up to a maximum of 10 percent by volume (E10). The emission inventory adjustment factors developed allowed for the modeling of ethanol blends up to 20 percent by volume (E20).

2. CONCEPT – CONCEPT is the on-road inventory processing software that was used to combine the inventory adjustment factors (noted above) with the pre-existing MOVES2010a inventories to yield scenario-specific inventories. CONCEPT was applied as part of CRC Project A-73-2.

3. SMOKE – Hydrocarbon (HC) speciation inputs were developed for use with EPA's Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system, which is software for preparing photochemical model inputs. Speciation data were developed for consistency with the on-road inventory approach for each fuel scenario evaluated. SMOKE was applied as part of CRC Project A-73-2 to integrate the speciation data into the development of photochemical model ready inventory inputs.

###

[2] This project used MOVES version 2010a (source code dated August 26, 2010) and underlying default database dated August 30, 2010.

2. DEVELOPMENT OF INVENTORY SCENARIOS

As noted above, emission inventories and speciation data were developed to reflect the emissions impacts associated with the use of distinct ethanol blends in on-road motor vehicles. The study domain was the lower 48 states of the United States and emission inventories at the county level. Emissions inventories and speciation data were developed for the four scenarios and calendar years listed below. It is important to note that the inventories for the 2005 and 2020 calendar years are impacted by changes in the vehicle fleet as well as the assumed fuels.

1. 2005 base year inventory, MOVES2010a default county fuel assumptions
2. 2020 future year inventory reflecting nationwide E10 usage
3. 2020 future year inventory reflecting nationwide E15 usage
4. 2020 future year inventory reflecting nationwide E20 usage

The 2005 inventory represents a base year in which ethanol use was based on historical fuel data for each county as specified in the default assumptions of the U.S. EPA MOVES2010a emissions model. The E10 scenario reflects nationwide use of E10 in all vehicles; the E15 and E20 scenarios assume use of those fuels only in 2001 and later model-year vehicles, with the remainder of the fleet assumed to be operating on E10.

2.1 Assumed Gasoline Properties

Based on extensive research, it has been determined that vehicular emissions are affected by the properties of the fuels on which they operate, and mathematical relationships between fuel properties and emissions have been developed by regulatory agencies and others. Ethanol content is one of these fuel properties; however, ethanol content can also affect other fuel properties. In order to develop emission inventory and speciation data for purposes of this project, it was necessary to make assumptions regarding these other fuel properties.

For the 2005 base year, MOVES2010a defaults were retained as the scenario gasoline properties (which are described in Section 2.2.2). For the 2020 fuel scenarios, Table 2-1 summarizes the assumed gasoline properties (as derived by CRC members) for E10, E15,

and E20 blends. For 2020, fuel properties were assumed to be uniform across the U.S. (i.e., no geographic variation) and reflected maximum marketshare penetration.[3]

Table 2-1
2020 Scenario Gasoline Properties by Ethanol Blend

	Summer Season Gasoline			Winter Season Gasoline		
Gasoline Parameter	E10	E15	E20	E10	E15	E20
RVP, PSI	7.8	7.8	7.8	10.3	10.3	10.3
Sulfur Level, ppm	30	30	30	30	30	30
Ethanol, Volume %	10	15	20	10	15	20
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, %	27.4	25.8	24.3	20.6	19.3	18.2
Olefin Content, %	7.5	7.1	6.6	11.5	10.8	10.2
Benzene Content, %	N/D	N/D	N/D	N/D	N/D	N/D
T50 (degrees F)	205	166	163	181	161	161
T90 (degrees F)	329	325	323	324	320	318

2.2 MOVES2010a Treatment of Fuel Properties

MOVES2010a includes default fuel formulation data by county, year, and month representing geographically resolved in-use gasoline. The data used by the model for 2005 and 2020 gasoline (both summer and winter formulations) were extracted from the model and incorporated into the modeling approach to develop inventory adjustment factors. Moreover, the model default fuel assumptions were also used as the scenario fuel assumptions for the 2005 base year scenario (as described above).

Noteworthy comments on these data are outlined below.

1. January and July data were extracted to represent winter and summer season fuels for each calendar year.

2. The 2005 default data include up to four separate formulations for each county and a fractional marketshare for each (with most counties represented by one or two formulations). Various oxygenates are present, including ethanol and MTBE as well as oxygenate-free gasoline.

[3] For the E15 and E20 fuel scenarios, 100% of 2001 and later model year vehicles were assumed to operate on the E15 and E20 formulations, with the remaining on-road and non-road fleet operating exclusively on E10.

3. For the 2020 default data, the model's fuel input databases include gasoline parameters by county projected to 2012, and properties are held constant thereafter for evaluating subsequent calendar years. Therefore, 2020 default gasoline properties used by the model are those carried forward from 2012. The default 2020 data include only one formulation per county (either ethanol-free or E10); the overall E10 marketshare (48-state average) is 90% in these defaults. It was also noted that the use of E0 was limited to portions of 10 states (mostly in the southeastern U.S.), with the remaining 38 states at 100% E10 use).

MOVES2010a estimates fuel corrections (defined as a multiplicative adjustment to emissions) relative to a specific reference fuel. The properties defining the MOVES2010a reference case gasoline are shown in Table 2-2. Fuel corrections developed are always calculated in relative terms and are therefore explicitly defined relative to the properties that define this case.

Table 2-2
MOVES2010a Reference Case Gasoline Properties
(MOVES Fuel Correction Factor = 1.0)

Gasoline Parameter	Value
RVP, PSI	6.9
Sulfur Level, ppm	30
Ethanol, Volume %	0
MTBE, Volume %	0
ETBE, Volume %	0
TAME, Volume %	0
Aromatic Content, %	26.10
Olefin Content, %	5.60
Benzene Content, %	1.00
E200, %	41.10
E300, %	83.10

Given the specification of fuels properties in Table 2-1 and the fuel properties used in the MOVES2010a model, it was necessary in the course of this project to convert between distillation points (i.e., T50 and T90) and evaporation points (i.e., E200 and E300).[4] Given that MOVES2010a already incorporates the formulas shown below to make these conversions, those formulas were used here.

[4] T50 and T90 define the respective temperatures at which 50% and 90% of gasoline is evaporated. E200 and E300 define the percent of fuel evaporated at the respective temperatures of 200°F and 300°F.

MOVES2010a T50/E200 and T90/E300 Conversions

$$T50 = 2.0408163 \times (147.91 - \text{E200})$$
$$T90 = 4.5454545 \times (155.47 - \text{E300})$$

In addition, because MOVES2010a uses oxygen content (in units of weight percent) in various calculations related to fuel correction factors, it contains the equation shown below for converting from fuel ethanol content on a volumetric basis to fuel oxygen content on a weight basis. This conversion was also used in this study.

MOVES2010a Oxygen/Ethanol Content Conversion

$$Oxygen_{EtOH}(Wt.\%) = 0.3488 \times Ethanol(Vol.\%)$$

2.3 Data Sets Developed for Use in Air Quality Modeling

As noted above, it was necessary to provide both emission inventory adjustments as well as speciation data for use in the air quality modeling performed as part of the A-73-2 project. This was done by providing two distinct data sets: inventory adjustment factor inputs, and speciation data inputs. Eight data sets were developed (4 scenarios and 2 seasons) covering the 3,110 counties in the lower 48 states (those distinguished by unique Federal Information Processing Standard or FIPS codes in MOVES2010a).

Inventory adjustment factors account for changes in mass emissions for each scenario and season combination relative to the MOVES2010a reference case. These data were reported for hydrocarbons (HC), carbon monoxide (CO), oxides of nitrogen (NOx) and particulate matter of 2.5 micrometers or less in diameter ($PM_{2.5}$) resolved by vehicle class, model year, and emissions process. The development of the inventory adjustment factors is described in Section 3 of this report.

Chemical speciation data were compiled to convert aggregate HC inventory results into the class of species defined by the Carbon Bond mechanism, version 5 (or CB05). This conversion to CB05 species is required to support photochemical modeling. HC speciation profiles were updated for consistency with the HC inventory methodology and ethanol content of each fuel scenario. The development of the speciation data is described in Section 4 of this report.

###

3. DEVELOPMENT OF INVENTORY ADJUSTMENT FACTORS

3.1 Overview

County-level inventory adjustment factors were developed for the application to preexisting national on-road emission inventories for 2005 and 2020 (with separate summer and winter season results). The preexisting inventories represent those of the MOVES2010a model under model default fuel assumptions for 2005 and 2020. The inventory adjustment factors were developed for application as a post-model adjustment. The adjustment factors were developed for the four fuel scenarios, and assumed gasoline properties are those defined in Section 2.

Outlined below are the emission processes for which inventory adjustment factors were developed.

1. Exhaust: The fuel correction factor method was updated for 2001 and newer model year passenger cars and light-trucks, and adjustment factor results reflect fuel scenario assumptions including blends up to E20.

2. Evaporative permeation: The fuel correction factor method was updated for 2001 and newer model year passenger cars and light-trucks, and results reflect fuel scenario assumptions including blends up to E20.

3. Evaporative/refueling vapor: Adjustment factors were developed to account for the RVP change on gasoline vapor emissions (as defined by the scenario gasoline properties) using the existing MOVES2010a methods.

For the 2005 base year scenario, only exhaust and evaporative permeation adjustment required calculation (methodology change only); for the 2020 scenarios, adjustment factors for all three processes required calculation (both methodology and fuel parameter changes).

The development of the exhaust, evaporative permeation, and evaporative/refueling vapor adjustment factors are described individually below, followed by a discussion of the results from this evaluation.

3.2 Exhaust

Exhaust emissions adjustment factors were developed for 2001 and newer model year light-duty gasoline cars and trucks and were defined for total organic gases (TOG,) volatile organic compounds (VOC), CO, NOx and PM species. The adjustment factors for this sector of the on-road fleet incorporated new fuel correction methods for late model year vehicles and addressed the range of ethanol content from 0% to 20% by volume.[5] The new fuel correction methods are based on predictive model[6] equations from the exhaust data collected under the EPAct test program, as developed by Richard Gunst for the U.S. Department of Energy.[7]

Initially, separate adjustment factors were considered for startup and running exhaust processes. However, for a number of reasons, it was ultimately decided that the use of composite test results was the most appropriate basis for the development of fuel adjustment factors which resulted in the same adjustments being applied for startup and running exhaust.

Before proceeding, it is important to note, as discussed in Section 2, that the sulfur content of gasoline was assumed to be the same for all scenarios and to be the same as the level assumed in the MOVES2010a default gasoline properties. This is significant because MOVES2010a adjusts for sulfur in gasoline separately from the other fuel adjustments, and accounting for sulfur changes would have added another level of complexity in the development of the fuel correction method.

Specifically for the exhaust adjustment factor method, the analysis replaced the preexisting fuel correction method of MOVES2010a with those developed from the EPAct test program for the targeted model year light-duty fleet. The exhaust adjustment factor was calculated as the ratio of two separate adjustment factors (both defined as multiplicative adjustment factors): the EPAct-based adjustment factor (numerator) and the MOVES2010a adjustment factor (denominator), as shown below.

Equation 1

$$Exhaust\ AF = \frac{EPAct\ Exhaust\ AF}{MOVES2010a\ Exhaust\ AF}$$

[5] Exhaust inventory adjustment factors were not developed for older model year light-duty vehicles, motorcycles, or heavy-duty gasoline vehicles; therefore, the fuel adjustment inherent in the preexisting MOVES2010a inventories were retained without modification.

[6] The term "predictive model" is used as a generic term in this document and is not meant to signify a particular model (i.e., the California Air Resources Board's Predictive Model). Actual model names, when referenced, are capitalized in this document.

[7] "Statistical Analysis of the Phase 3 Emissions Data Collected in the EPAct/V2/E89 Program," National Renewable Energy Laboratory Subcontract No. LGC-0-40441-01, Principal Investigator: Richard F. Gunst, Final Report, July 1, 2011.

Key specifics of this approach are summarized below.

- The MOVES2010a adjustment factor is that used in the preexisting inventory. It is the exhaust correction for the MOVES2010a default properties (by county, season, and year) defined relative to MOVES2010a reference gasoline, where MOVES2010a default and reference gasoline properties are described in Section 2.2. Applying this factor in the denominator of Equation 1 removes the preexisting MOVES2010a fuel corrections in the application of the exhaust adjustment factor.

- The EPAct adjustment factor, applied in the numerator of Equation 1, is defined as the multiplicative factor to adjust the exhaust inventory for fuel scenario conditions as calculated relative to the MOVES2010a reference gasoline. Scenario and reference gasoline properties are described in Section 2.

- For 2005 MOVES2010a default gasoline parameters (as noted in Section 2), multiple gasoline formulations and oxygenate types are possibly present (for a given county). The exhaust factor calculation was completed for each formulation separately (when multiple formulations were present), and the final exhaust factor for the county was the combination of the formulation-specific exhaust adjustment factors (defined by Equation 1) combined in proportion to the marketshare of each formulation.[8]

- For the 2020 MOVES2010a default gasoline properties, there is only one formulation of gasoline assigned to each county—either E0 (ethanol free) or E10—and handling of multiple formulations was not required for completing the 2020 fuel scenarios.

Both the EPAct and MOVES2010a exhaust adjustment factors shown in Equation 1 were estimated from predictive model equations that share common features, as illustrated in Equation 2. The predictive models were developed from linear regressions of fuel variables and combinations of fuel variables, completed in logarithmic space. The predictive model equations produce estimated emission factors (typically in the units of g/mi) represented by the generic formula shown below, where the summation is over the specific number of variable-and-coefficient combinations contained in the specific predictive model used.[9]

[8] Note that the exhaust adjustment factor approach and supporting data described herein address only ethanol free (E0) gasoline (with no other oxygenate present) and ethanol blends up to E20. For ether-based oxygenates in gasoline still in use in 2005, the exhaust adjustment factor defined by Equation 1was assigned to unity (no change in emissions) wherever applicable, meaning that ether-based oxygenate fuel corrections were retained without modification from what is assumed by MOVES2010a.

[9] "exp" refers to the exponential function in Equation 2. "Variable" in Equation 2 can be expressed as the actual variable value (in absolute terms), or it can be expressed as the standardized value of the variable (as defined by Equation 2).

Equation 2

$$predictive\ model\left(\frac{g}{mi}\right) = \exp\left(Intercept + \sum Coefficien\,t \times Variable\right)$$

In the application of the predictive models, the exhaust adjustment factors were determined by the ratio of the emission factor prediction at the target fuel conditions over the emission factor prediction at the reference fuel conditions (i.e.,, MOVES2010a reference gasoline, see Table 2-2). In this way, the predictive model emission factors were used in relative terms for this project (to estimate relative fuel effects), not in absolute terms.

For some predictive models, the underlying variables (e.g., gasoline properties) are defined in absolute terms, but for most predictive models, the variables are defined in standardized terms. The standardization of an input variable, when applicable, is generically defined as follows:

Equation 3

$$Standarized\ Varaible = \frac{Variable - Mean}{Standard\ Deviation}$$

In Equation 3, the "variable" is the absolute value for the modeling variable used as input into the predictive model, whereas the "mean" and "standard deviation" are the statistical mean and standard deviation from the set of fuel variables used in the underlying predictive model development.

The remainder of this discussion describes the two parts of the exhaust adjustment factor calculation separately (the EPAct adjustment factor and the MOVES2010a adjustment factor defined in in Equation 1), as the underlying methods are distinct. Included are the details of each predictive model used.

3.2.1 EPAct Exhaust Adjustment Factors

The EPAct exhaust adjustment factors were based on the predictive model equations developed by the DOE-sponsored study (referenced in footnote 7). The EPAct testing was completed for 27 test fuels (E0 to E20) with 15 Tier 2 certified light-duty vehicles. Specific assumptions and details are outlined below.

1. The "benchmark" equations were used to develop adjustment factors (both benchmark and simplified forms of the predictive models were developed). The benchmark model represents the coefficients defined by retaining all fuel variables.

2. The FTP-composite equations were used (both composite and bag-specific models were developed). As a result, the running and startup exhaust adjustment factors were equivalent.

3. The 2001 and newer model year light-duty fleet was modeled as a single group without further distinctions by the equations developed.

4. The predictive model results in g/mi emission factors, except for PM exhaust (units of mg/mi).

Table 3-1 presents the list of the 17 fuel variables making up the predictive models used. The modeling coefficients for each variable and the values (i.e., means and standard deviations) used to calculate standardized fuel variables are listed for the pollutants that were used for adjustment factor development. The values for standardization reported here were obtained directly from the Principle Investigator as they were not included in the original source reference (see footnote 7).[10]

EPAct exhaust adjustment factors were calculated by the ratio of emissions factors predicted from these equations (i.e., the emission factor with scenario properties over the emission factor with reference gasoline properties). Key specifics and assumptions in these calculations are summarized below.

1. Gasoline property assumptions were those described in Section 2.

2. Note that the equations, developed from the 27 EPAct fuels, are based on a maximum RVP specification of 10.3 PSI. An analysis of winter season correction factors was completed and ultimately it was determined that the equations should not be extrapolated beyond the 10.3 limit despite the fact that the average winter RVP value initially provided by CRC was 12.6 PSI. Accordingly, the winter season scenario gasoline properties were explicitly capped at 10.3 PSI in their final form.

3. Adjustment factors expressed as TOG were calculated from the combined results of NMOG plus CH_4.

4. Adjustment factors expressed as VOC directly relied on the NMOG equations as the nearest match to VOC.

[10] Note that the cross product and squared variables used are calculated from standardized values of the fuel parameters from the 27 EPAct test fuels; the mean values reported therefore centered around zero.

Table 3-1
Predictive Models for Calculating EPAct Exhaust Adjustment Factors

	Modeling Coefficients and Intercept by Exhaust Pollutant					Standardization Parameter Values	
Variable	NMOG	CH4	CO	NOx	PM	Mean	Standard Deviation
Intercept	*-3.6493*	*-5.0354*	*-0.6456*	*-4.3549*	*-0.70961*	*N/A*	*N/A*
T50	0.1405	0.08344	0.03311	0.01621	-0.0352	190.6111	28.5791
T90	0.0356	0.01802	-0.0419	0.00584	0.1611	320.5333	19.4801
RVP	0.09173	0.07912	-0.02842	0.06761	0.0836	10.3137	7.8796
ARO	-0.04453	-0.0146	0.02456	0.02697	-0.0849	8.5178	1.6114
EtOH	0.09348	-0.09512	0.05817	0.06656	0.2663	25.6296	10.0154
T50*T50	0.08048	0.03815	0.04222	0.02209	-0.0082	0.9630	0.7398
EtOH*EtOH	0.03918	0.02056	0.05984	0.00517	-0.0832	0.9630	0.8028
T90*T90	0.0111	-0.00662	0.00743	-0.00627	0.1184	0.9630	0.3470
T50*T90	0.04613	0.01549	0.02533	0.02014	0.1023	-0.0363	0.9600
T50*EtOH	0.0344	0.01609	0.0599	0.0078	-0.1247	-0.5413	0.7692
T50*ARO	0.01693	0.02377	0.03226	0.06477	-0.0396	-0.0680	0.9917
T90*EtOH	0.03776	0.01054	0.02322	0.01798	0.1039	0.0163	0.9728
T90*RVP	-0.01306	-0.00483	0.01302	0.00326	-0.0308	0.1268	0.9727
T90*ARO	0.01917	0.01705	0.01892	-0.01671	0.0763	-0.0063	0.9835
EtOH*RVP	-0.00004	-0.00236	-0.00143	-0.00152	-0.0326	-0.0992	0.9996
EtOH*ARO	0.03691	0.03087	0.03843	0.0298	0.0701	-0.0367	0.9785
RVP*ARO	0.02973	0.02407	0.02615	0.03497	-0.0418	0.0438	0.9841

Note: EtOH = ethanol volume %; ARO = aromatic content (%)

3.2.2 MOVES Exhaust Adjustment Factors

The MOVES exhaust adjustment factors are those preexisting model fuel corrections for 2001 and newer model year light-duty vehicles that were factored out of the inventory as the denominator of the exhaust adjustment factor equation (Equation 1). The MOVES exhaust adjustment methods are distinct for HC, NOx, and CO; the correlations used to evaluate these three pollutants are described individually below. For all three pollutants, the model's adjustment factors are based on FTP-composite equations and resulting factors are equivalent for both running and startup exhaust. The MOVES2010a exhaust adjustment factor for PM is unity in all instances (the model applies no fuel corrections to PM exhaust other than sulfur), and PM is not described further in this discussion of MOVES2010a adjustment factors.

For exhaust HC and NOx exhaust fuel corrections, MOVES2010a is based on the predictive models that EPA developed for the 2001 review of the California ARB oxygenate waiver request.[11] These were developed from Tier 0 vehicle FTP-composite test data and are applied in MOVES2010a for all model year vehicles up to model year 2003 (after which the exhaust HC and NOx fuel corrections of MOVES2010a are unity).[12] There are multiple predictive models defined for both pollutants (from the same underlying set of data): three for NMHC and six for NOx. Each model is used to predict a g/mi emission rate, and the final g/mi emission rate is estimated by a simple average over all models. The MOVES2010a predictive model coefficients and standardizing parameters are shown in Table 3-2 and 3-3 for NMHC and NOx, respectively. Note that the enumeration of models shown in Tables 3-2 and 3-3 (e.g., "Model 7" of Table 3-2) is specifically EPA's model labeling scheme and is non-sequential because EPA developed more model versions than were ultimately selected for use in fuel effects modeling.

For CO exhaust, MOVES2010a is based on the predictive models that EPA developed for the specialized CO-version of the Complex Model, in which the equations were developed from Tier 0 vehicle FTP-composite test data. There are multiple technology distinctions within the CO predictive models programmed into MOVES, based on separating the underlying data by fuel metering/catalyst technology and high emitter status.[13] For the 2001 and newer model years, MOVES2010a relies on three separate CO predictive models (this model year group is treated as a whole):

- Model 1 = "PFI & 3way & No Air & EGR" (normal emitting);
- Model 4 = "PFI & 3way+Ox & Air & EGR" (normal emitting); and
- Model 10 = "All High Emitters."

The weight factors for combining these three technology models are a function of age (but not vehicle class). High emitters range from 1.9% (age =0) to 32.8% (age = 30). The normal emitters (those that are not high emitters) are split at 75% and 25% for Models 1 and 4, respectively.[14] The MOVES2010a predictive model coefficients and standardizing parameters for exhaust CO are shown in Table 3-4.[15]

[11] "Technical Support Document: Analysis of California's Request for Waiver of the Reformulated Gasoline Oxygen Content Requirement for California Covered Areas United States," Environmental Protection Agency, Office of Air and Radiation, EPA420-R-01-016, June 2001.
[12] A fuel correction factor of unity signifies that no fuel effects are modeled in MOVES2010a for HC and NOx exhaust for all model years 2004 and newer. The exception to this is for fuel sulfur corrections, which are handled separately from the remaining fuel property corrections.
[13] "MOVES2010 Fuel Adjustment and Air Toxic Emission Calculation Algorithm – Development and Results," U.S. Environmental Protection Agency, EPA-420-R-11-009, July 2011.
[14] Although the predictive model equations themselves originate from the CO version of the Complex Model, the weight factors for the individual predictive are specific to MOVES2010a (and do not equal those weight factors of the Complex Model).
[15] For the MOVES2010a CO predictive models, intercepts are not calculated (i.e., equivalent to zero), and standard deviations are not used to standardize input variables (i.e., equivalent to unity).

Table 3-2
Predictive Models for Calculating MOVES2010a Exhaust Adjustment Factors
NMHC Exhaust, 2001-2003 Model Years Only

	Modeling Coefficients and Intercept for Three Separate Predictive Models			Standardization Parameter Values	
Variable	Model 7	Model 8	Model 12	Mean	Standard Deviation
Intercept	*-1.5957*	*-1.5980*	*-1.6012*	*N/A*	*N/A*
RVP	0.008474	0.008971	0.007973	8.51	0.781459
T50	0.06125	0.06499	0.06046	205.62	17.612534
T90	0.02084	0.02104	0.02133	310.65	20.869732
ARO	0.008729	0.008465	0.008759	27.64	6.561886
OLE	-0.01426	-0.01430	-0.01457	6.93	5.143184
OXY	-0.01329	-0.01378	-0.01391	1.49	1.249356
SUL	0.05505	0.05495	0.04696	183.14	143.055894
HIGH	1.6909	1.6935	1.7091	(a)	
T90*T90	0.01617	0.01604	0.01633	(b)	
T50*T50	0.02494	0.02477	0.02469		
T90*OXY	0.01589	0.01576	0.01552		
SUL*HIGH	-0.03174	-0.03172			
OXY*OXY	0.01256	0.01353	0.01288		
T90*ARO	0.006908	0.007013	0.006814		
T50*HIGH		-0.02609			

Note: ARO = aromatic content (%); OLE = olefin content (%); OXY = oxygen weight %; SUL = sulfur content (ppm); HIGH = high emitter fraction

(a) The standardized input value for HIGH always equals 1 in the application of the HC and NOx predictive models within MOVES2010a. This means that high emitter proportions do not change from those inherent in predictive model equations based on their original development.

(b) Means and standard deviations are not used to standardize the second-order variables (i.e., the cross product and squared terms). The standardized values for the cross-product and squared variables are mathematically determined from the standardized values for the first-order variables. For example, the standardized value for theT90*ARO term is the product of the standardized value for T90 times the standardized value for ARO.

Table 3-3
Predictive Models for Calculating MOVES2010a Exhaust Adjustment Factors
NOx Exhaust, 2001-2003 Model Years Only

Variable	Modeling Coefficients and Intercept for Six Separate Predictive Models						Standardization Parameter Values	
	Model 2	Model 3	Model 4	Model 5	Model 6	Model 7	Mean	Standard Deviation
Intercept	-0.6603	-0.6606	-0.6656	-0.6651	-0.6624	-0.6737	*N/A*	*N/A*
RVP	0.009093	0.01172	0.009694	0.007673	0.00839	0.006188	8.445335	0.780184
T50	-0.00245	0.000084	0.001804	0.001173	0.000312	-0.00475	206.8155	17.90627
T90	0.00719	0.007879	0.005543	0.006239	0.006213	0.007587	312.1262	22.09933
ARO	0.01587	0.01431	0.01524	0.01407	0.01501	0.01209	28.08281	7.383169
OLE	0.01988	0.01949	0.0194	0.01966	0.0199	0.01969	6.974371	4.932872
OXY	0.0124	0.01728	0.01333	0.01371	0.01351	0.008245	1.347629	1.251882
SULFUR	0.04171	0.04387	0.04201	0.04201	0.04195	0.04205	182.0603	140.7832
HIGH	0.396	0.3963	0.3965	0.396	0.3961	0.3969	(a)	
OXY*SUL	-0.01506		-0.01647	-0.01627	-0.01402	-0.01325	(b)	
OXY*T50				-0.0083				
OXY*T90		-0.0051						
OXY*ARO					-0.00547			
OXY*OXY						0.0112		
T50*T50			0.006974					

Note: ARO = aromatic content (%); OLE = olefin content (%); OXY = oxygen weight %; SUL = sulfur content (ppm); HIGH = high emitter fraction

(a) The standardized input value for HIGH always equals 1 in the application of the HC and NOx predictive models within MOVES2010a. This means that high emitter proportions do not change from those inherent in predictive model equations based on their original development.

(b) Means and standard deviations are not used to standardize the second-order variables (i.e., the cross product and squared terms). The standardized values for the cross-product and squared variables are mathematically determined from the standardized values for the first-order variables. For example, the standardized value for theT90*ARO term is the product of the standardized value for T90 times the standardized value for ARO.

Table 3-4
Predictive Models for Calculating MOVES2010 Exhaust Adjustment Factors
CO Exhaust, 2001 and Newer Model Years

Variable	Modeling Coefficients for 3 Technology-Specific Predictive Models			Standardization Parameter
	Model 1	Model 4	Model 10	Mean
OXY	-0.032584	-0.095314	-0.019006	1.774834
SUL	0.000419	0.000919	0.000419	204.5779
RVP	0.043314	0.003448	0.003448	8.611479
E200	-0.002335	0.005751	-0.002335	46.72577
E300	0.002372	0.002372	0.002372	85.8962
ARO	0.007795	0.00547	0.00547	28.26109
OLE	0.000507	0.000507	0.000507	7.318716
RVP*RVP	0.017288	0.007093	0.007093	17.22296
E200*E200	7.76E-05	7.76E-05	7.76E-05	93.45154
E300*E300	0.000515	0.000515	0.000515	171.7924
OLE*OLE	0.000291	0.000605	-0.000104	14.63743
E300*OLE	0.000362	0.000362	0.000362	628.6499

Note: OXY = oxygen weight %; SUL = sulfur content (ppm); ARO = aromatic content (%); OLE = olefin content (%)

For all three pollutants, MOVES exhaust adjustment factors for this evaluation were calculated by ratio of emissions factors predicted from the equations documented in Tables 3-2, 3-3, and 3-4. Each adjustment factor is defined as the ratio of the predicted rate from the default MOVES2010a fuel variables (by season and by county) over the rate for the reference gasoline variables, following the gasoline parameter assumptions defined in Section 2.2. These calculations form the basis of the denominator shown in Equation 1.

Finally, the reporting of HC exhaust adjustment factors as either TOG or VOC requires further calculations that are fuel-specific. The predictive models for HC exhaust are in the form of NMHC (as shown in Table 3-2). Equations 4 and 5 convert HC exhaust adjustment factors from NMHC over to TOG or VOC, and are a function of ethanol content (defined by oxygen weight percent).

Equations 4 and 5

$$MOVES\ Exhaust\ AF\ (TOG) = MOVES\ Exhaust\ AF\ (NMHC) \times \frac{1.0163 + 0.0062 \times Oxygen_{EtOH}\ (Wt.\%)}{1.0163}$$

$$MOVES\ Exhaust\ AF\ (VOC) = MOVES\ Exhaust\ AF\ (NMHC) \times \frac{0.9797 + 0.0133 \times Oxygen_{EtOH}\ (Wt.\%)}{0.9797}$$

These equations represent a simplified case over the more general equations used by MOVES2010a (as documented in the reference cited in footnote 13). Specifically, the equations incorporate the assumptions that the reference gasoline case is ethanol free and that methane in MOVES2010a is treated as a proportional fraction of THC exhaust (i.e., methane cancels out of the adjustment equations between HC-reporting bases as applied in this evaluation).[16]

3.3 Evaporative Permeation

The evaporative permeation adjustment factors were developed for 2001 and newer model year light-duty gasoline cars and trucks. The adjustment factors for this sector of the on-road fleet incorporated new test data over a range of ethanol content from 0% to 20% by volume.[17] The permeation adjustment factors are defined for TOG and VOC and are based on the compilation of CRC test programs (Projects E-65 and E-77).[18] The only gasoline parameter impacting permeation emission rates is ethanol content, where permeation emissions increase for gasoline that includes ethanol when compared to ethanol-free gasoline.

Specifically for the evaporative permeation adjustment method, the analysis replaced the preexisting fuel correction method of MOVES2010a with those developed for this evaluation. The permeation inventory adjustment factors developed were then calculated as the ratio of two separate adjustment factors (both defined as multiplicative adjustments): the updated permeation adjustment factor (numerator) and the MOVES2010a adjustment factor (denominator), as shown below.

[16] MOVES2010a is designed such that methane is calculated as a multiplicative fraction of THC where the methane fraction does not have a fuel variable dependence. As a consequence, the fuel corrections of MOVES2010a are mathematically equivalent for HC exhaust reported as THC, NMHC or methane.

[17] Adjustment factors were not developed for older model year light-duty vehicles, motorcycles, or heavy-duty gasoline vehicles; therefore, the fuel adjustments inherent in the preexisting MOVES2010a inventories were retained without modification.

[18] Evaporative permeation adjustments are defined as multiplicative adjustments (where unity represents no change in emissions). Permeation adjustments are equivalent when expressed as either TOG or VOC.

Equation 6

$$Permeation\ AF = \frac{Updated\ Permeation\ AF}{MOVES2010a\ Permeation\ AF}$$

The adjustment factors of Equation 6 are defined relative to the MOVES2010a reference gasoline, which contains no ethanol (see Section 2.2). Adjustment factors for gasoline without ethanol are 1.0 by definition.

Both the MOVES2010a and the updated adjustment factor methods of Equation 6 are based on CRC test program data from Projects E-65 and E-77. Differences between updated and MOVES2010a permeation methods are summarized below.

- MOVES2010a includes E-77 results only through project E-77-2b; the updated method includes E-77 results through project E-77-2c.

- MOVES2010a includes ethanol blends only up to 10% by volume; the updated method included ethanol blends up to 20% by volume.

- The MOVES2010a method treats all vehicles meeting enhanced evaporative standards and Tier II/LEV II evaporative standards as one group; the updated method found distinct impacts for enhanced evaporative and Tier II/LEV II evaporative standards.

For these reasons, the two methods result in different evaporative permeation adjustment factors.

In terms of the MOVES2010a adjustment method (denominator of Equation 6), the ethanol impact on permeation from all light-duty vehicles meeting enhanced, Tier II, and LEV II evaporative standards is handled by a single factor. The multiplier 2.1383 is applied by the model to adjust any E0 fuel to a low-level ethanol blend (up to 10% by volume) where the adjustment does not vary by ethanol content. This single factor therefore encompasses all 2001 and newer model year light-duty gasoline vehicles of interest to this evaluation.

In terms of the updated permeation method (numerator of Equation 6), the ethanol impact on permeation was updated to incorporate new test data and to examine the consequences of mid-level ethanol blends. Details of the updated permeation adjustment factor development are outlined below.

- Vehicles from the CRC test programs were grouped by evaporative standard. For 2001 and newer model years, three sets of standards are applicable: enhanced, Tier II or LEV II "near zero," and LEV II "zero" evaporative standards. In the final form, the method combined the near-zero and zero evaporative standards

into one group, which was used to model permeation effects for 2004 and newer model year vehicles. The data for vehicles meeting enhanced evaporative standards were used to update model permeation effects for 2001 to 2003 model year vehicles.

- Results from both static and dynamic permeation tests were used. Results were corrected to a common 86°F so that all test types could be utilized.[19]

- Results were stratified by individual ethanol blend level tested (E0, E6, E10 and E20). Permeation emission rates were significantly higher for all three ethanol blends relative to E0. Permeation emission rates for ethanol blends were statistically similar (E6, E10, and E20); permeation rates for E0 were statistically different from ethanol-containing blends. Therefore, a single permeation adjustment was developed that encompasses all ethanol blends up to 20% by volume and is defined relative to E0.

- For 2001 to 2003 model years (i.e., enhanced evaporative standards), two of the three-day dynamic tests were removed because the day-to-day variation over three days was questionable.[20] A total of 124 tests from 12 vehicles were used to define mean permeation rates for E0 and ethanol blends of 18.80 and 40.81 g/hr (at 86°F), respectively. These results equate to an updated permeation adjustment factor of 2.16 for ethanol blends (ethanol blend divided by E0).

- For 2004 and newer model years (i.e., Tier II and LEV II standard), a total of 80 tests from 7 vehicles were used to define mean permeation rates for E0 and ethanol blends of 6.83 and 11.90 g/hr (at 86°F), respectively. These results equate to an updated permeation factor of 1.75 for ethanol blends (ethanol blend divided by E0).

Overall, Equation 6 was applied in this study as follows: the updated permeation factors of 2.16 and 1.75 for 2001-2003 and for 2004 and newer model years, respectively, were applied for any scenario gasoline with ethanol; the MOVES2010a permeation factor of 2.1383 was applied for anyMOVES2010a default gasoline with ethanol.

[19] Exponential temperature corrections were developed using the static test results at 86°F and 105°F. Analyses showed that once corrected to a uniform temperature, static and dynamic permeation results were statistically similar.

[20] Multi-day dynamic tests were included in both E-65 and E-77 covering either two- or three-day periods, with permeation rates remaining statistically similar from day-to-day in all but 2 instances. The two tests removed had third-day permeation rates that were in excess of 15 times the permeation rates measured on the first day.

3.4 Evaporative /Refueling Vapor

Separate evaporative and refueling vapor emissions adjustments were developed for each class of gasoline-powered vehicle to address the single fuel variable of RVP. Unlike exhaust and permeation adjustment factors, the methods for vapor adjustment factors described herein are those of MOVES2010a without significant modification.

The RVP-based adjustment to evaporative and refueling vapor emissions was required to be calculated for this evaluation only when the RVP specification of the fuel scenario differed from the preexisting MOVES2010a default. As described in Section 2.2, there is no difference in fuel assumptions for the 2005 base year scenario (and no vapor emission correction factors were calculated). For the three 2020 fuel scenarios, vapor emission adjustment factors were developed for the RVP specifications assumed in each scenario.

The vapor emissions adjustment factor took the form of the following equation:

Equation 7

$$Vapor\ AF = \frac{Vapor\ Rate\left(Scenario, \frac{g}{vehicle}\right)}{Vapor\ Rate\left(MOVES2010a, \frac{g}{vehicle}\right)}$$

In Equation 7, "Scenario" refers to the RVP of the modeling scenario and "MOVES2010a" refers to the MOVES2010a default RVP (by county by season). Generally speaking, vapor emissions increase with increasing RVP. Specifics of developing adjustment factors for the 2020 fuel scenarios are provided below.

- For the 2020 scenarios, the scenario RVP is either 7.8 or 10.3 PSI (for summer and winter seasons, respectively), as shown in Table 2-1. Equation 7 was applied to determine the vapor emissions adjustment factors to correct the inventory to the uniform seasonal scenario RVP assumption.

- For the 2020 MOVES2010a summer season defaults, the RVP ranges from 6.9 to 9.7 PSI. For those counties with RVP below 7.8 PSI, the vapor adjustment factor was greater than one and the vapor emissions increased under the scenario conditions. Conversely, for those counties with RVP above 7.8 PSI, the vapor adjustment factor was less than one.

- For the 2020 MOVES winter season defaults, the RVP ranges from 9.8 to 15.3 PSI. For those counties with RVP below 10.3 PSI, the vapor adjustment factor calculated was greater than one and the vapor emissions increased under

the scenario conditions.[21] Conversely, for those counties with RVP above 12.6 PSI, the vapor adjustment factor was less than one.

Estimating the vapor emission rates for Equation 7 was completed through a simplified process because the MOVES2010 methods reflect a complex relationship defining tank temperature that could not be easily handled in a post-model correction.[22] The simplified process entailed using MOVES2010a (under national default conditions by season for fleet mix, operation characteristics, and temperature profiles) to estimate per-vehicle vapor generation rates as a function of RVP. Details of this vapor rate estimation method were as follows:[23]

- Vapor rates were defined separately for evaporative vapor and refueling vapor emissions;
- Vapor rates were defined separately for each gasoline-powered vehicle class (PC, LDT, HDV, and MC);
- Seasonal vapor rates were defined by operating MOVES2010a for the range of 6.5 to 15.5 PSI in increments of 0.5 PSI and then normalized such that the vapor generation rate at 6.5 PSI equaled unity; and
- Polynomial curve fits were defined so that the vapor rates could be modeled as a continuous function. The vapor rate functions were defined as second-order polynomial curves as shown in Equation 8 with the coefficients listed in Table 3-5.

Equation 8

$$Vapor\ Rate = A \times RVP + B \times RVP^2 + C$$

[21] Winter season areas with RVP below 10.3 PSI include areas of the southwest U.S. that have winter season RVP caps.
[22] MOVES2010a vapor generation algorithms are a function of ambient temperature and a distribution of driving patterns; final emissions reported by the model are those from vapor generation not captured by the vehicle and refuel control systems. It was not feasible to replicate these calculations outside of the model.
[23] January and July conditions were used for winter and summer seasons, respectively.

Table 3-5 2020 Vapor Emission Rate Equation Coefficients				
		Equation Coefficients		
Process and Season	Vehicle Class	A	B	C
Evaporative Vapor, Summer	HDV	-0.4793	0.0328	2.8101
	LDT	-0.4924	0.0336	2.8603
	PC	-0.2534	0.0182	1.9185
	MC	-0.3822	0.0336	2.1161
Evaporative Vapor, Winter	HDV	-0.0540	0.0043	1.1793
	LDT	-0.0544	0.0043	1.1806
	PC	-0.0290	0.0024	1.0935
	MC	-0.1763	0.0149	1.5399
Refueling Vapor, Summer	HDV	0.1670	0.0000	-0.0856
	LDT	0.1670	0.0000	-0.0856
	PC	0.1668	0.0000	-0.0845
	MC	0.1676	0.0000	-0.0894
Refueling Vapor, Winter	HDV	-0.2163	0.0177	1.4883
	LDT	-0.2159	0.0177	1.4855
	PC	-0.2099	0.0175	1.4477
	MC	-0.2100	0.0175	1.4474

3.5 Results

The adjustment factor data were provided in electronic format. Eight datasets were developed (four scenarios and two seasons) covering the 3,110 counties in the lower 48 states (those distinguished by FIPS codes in MOVES2010a).[24] The data sets were provided in ASCII file format using comma-delimited records. Each record is defined by six fields of FIPS, vehicle class, model year, emission process, pollutant, and emission inventory adjustment factor.

The two seasonal data sets for the 2005 scenario contained 559,800 records each. The valid entries for each field are listed below.

- FIPS: 3110 distinct values from MOVES2010a
- Vehicle classes: "LDGV", "LDGT1", "LDGT2"
- Model years: 2001 through 2005 (inclusive)

[24] The 3,110 FIPS defined by MOVES includes Broomfield County, Colorado (FIPS=08014), which is unique. MOVES2010a has input data for this county, but the model does not produce emissions results. Because this county was created in 2003, the model cannot handle this case properly. Broomfield County was included in this evaluation for completeness.

- Processes: “RUNNING EXHAUST”, “START EXHAUST”, and “EVAP PERMEATION”
- Pollutants: “TOG”, “VOC”, “CO”, “PM”, “NOX”

The 2020 runs contained additional model years and processes, as described in the methodology. For the 2020 scenario data sets created, there were 1,256,440 records contained in each. Listed below are the valid entries for each field.

- FIPS: 3110 distinct values from MOVES2010a
- Vehicle classes: “LDGV”, “LDGT1”, “LDGT2”, “HDGV”, “MC”
- Model years: 2001 through 2020 (inclusive)[25]
- Processes: “RUNNING EXHAUST”, “START EXHAUST”, “EVAP PERMEATION”, “EVAP FUEL VAPOR”, “REFUELING VAPOR”
- Pollutants: “TOG”, “VOC”, “CO”, “PM”, “NOX”

The only adjustment factor results that raised concerns were those for PM exhaust in the 2005 scenario (using MOVES2010a default gasoline parameters). It was noted that, according to the predictive equations developed, the PM exhaust adjustment factor can exceed 2.0 when the T90 specifications for a given county exceeded those of the EPAct test program (maximum T90 of 341.8°F within the test program). The instances of this occurring were few—the states in which the fuel parameters caused the PM adjustment factor to exceed 2.0 were Texas, Nevada, Michigan, Maryland, and Pennsylvania, where PM exhaust emissions increase with T90 as per the equations.

###

[25] A model year value of “-9” was entered for the adjustment factors for evaporative vapor and refuel vapor processes that were not model year specific.

4. DEVELOPMENT OF HC SPECIATION INPUTS

4.1 Overview

Chemical speciation profile data were compiled to support the conversion of aggregate HC inventory results into the class of species defined by the Carbon Bond mechanism, Version 5 (or CB05).[26] This conversion of the HC inventory to CB05 species is required to support photochemical modeling. HC speciation was expressed in terms of total organic gases or TOG.

Updated TOG speciation profiles were developed in a manner consistent with the development of emission inventory adjustment factors for this project, as described in Section 3. In particular, the TOG speciation profiles developed represent the latest data on light-duty Tier 2 vehicles as well as the full range of ethanol blends up to 20% by volume as specified by the fuel scenarios under evaluation. Specifically, the speciation data were developed for the four fuel scenarios and the corresponding gasoline properties defined in Section 2.

TOG speciation profiles were developed for all gasoline on-road vehicle classes for each of the emission inventory processes. The datasets were formatted for use with EPA's Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system.[27]

4.2 Methods

The development of TOG speciation profiles included the use of the tools and resources described below.

1. SPECIATE is the EPA database or repository for HC and PM speciation profile data, updated periodically as new information becomes available. Version 4.2 was the public domain at the start of this evaluation, and an early release of Version 4.3 was provided for use in this project.[28] SPECIATE contains mass-based speciation profiles (the apportionment of the HC or PM inventory into

[26] "An Updated Photochemical Mechanism for Modeling Urban and Regional Air Quality: Carbon Bond, Version 5 (CB-V)," Systems Applications International, Inc. (SAI), ICF Consulting, December 4, 2002.
[27] SMOKE documentation and data formats are available at *http://www.smoke-model.org*.
[28] Both SPECIATE versions were publicly available at the time of publication of this report: *http://www.epa.gov/ttn/chief/software/speciate/index.html*.

individual chemical compounds). Each profile in SPECIATE is given a profile number, these indexing profile numbers were used in this evaluation as well to reference distinct profiles used.

2. Existing CB05-based speciation profile data (up through SPECIATE4.2) were utilized from the EPA's Emissions Modeling Clearinghouse (EMCH) website.[29] These data include SPECIATE 4.2 profiles converted into CB05 species and formatted for use with SMOKE.

3. Additional CB05-based speciation profile data were provided by Environ for use in this evaluation as they pertained to the newly defined speciation profiles of SPECIATE4.3 that were already prepared for EPA OAQPS.

4. The computer tool and documentation for converting mass-based speciation profiles over to CB05-based speciation profiles (developed by Environ) was provided by EPA OAQPS for this project.[30]

Development of the speciation profiles for the 2005 and 2020 scenarios is described separately below, as the methods for each are distinct.

4.2.1 2005 Base Year Scenario

For the 2005 base year, the SPECIATE profiles listed below were used in the scenario evaluation where the four-digit profile number is that of the SPECIATE database. Note that profiles 8756 and 8757 were based on speciated results from the EPAct test program.

- Profile 8750 was used for exhaust composite emissions (ethanol-free gasoline or E0) for pre-2001 model year light-duty vehicles and all model year heavy-duty vehicles and motorcycles.

- Profile 8751 was used for exhaust composite emissions (E10 gasoline) for pre-2001 model year light-duty vehicles and all model year heavy-duty vehicles and motorcycles.

- Profile 8756 was used for exhaust composite (E0) for 2001 and newer model year light-duty vehicles.

- Profile 8757 was used for exhaust composite (E10) for 2001 and newer model year light-duty vehicles.

- Profile 8753, representing an evaporative composite profile, was used for all evaporative processes with E0 gasoline.

[29] *http://www.epa.gov/ttn/chief/emch/speciation/index.html*.
[30] "Speciation Tool User's Guide, Version 2.0," Environ International Corporation, September 2007.

- Profile 8754, representing an evaporative composite profile, was used for all evaporative processes with E10 gasoline.

The speciation profiles developed for 2005 incorporate the scenario-specific marketshare of gasoline usage by ethanol blend (i.e., E0 and E10). The marketshare data varied by county in the scenario database (as discussed in Section 2.2) and, as such, the speciation profiles developed for the 2005 scenario vary by county in accordance with the underlying fuels used.

To incorporate the model year split in speciation profile assignment for light-duty vehicles, the fraction of emissions occurring from 2001 and newer model year light-duty vehicles was estimated for 2005 using MOVES2010a. The results, shown in Table 4-1, represent national default conditions by season for fleet mix, operation characteristics, and temperature profiles.[31] For example, the first value listed in Table 4-1 signifies that 20.0% of 2005 summer season exhaust composite TOG emissions from passenger cars (PC) comes from 2001 and newer model years; thereby the remaining 80.0% comes from 2000 and older model year PCs.

Table 4-1
Percent of 2005 TOG Emissions Occurring from 2001 and Newer Model Years
MOVES2010a, National Default Conditions

Emissions Process	PC, Summer	PC, Winter	LDT, Summer	LDT, Winter
Exhaust, Composite	20.0%	22.4%	5.9%	9.0%
Evaporative Permeation	6.0%	9.4%	6.0%	9.4%
Evaporative Vapor	4.9%	8.4%	4.5%	7.4%
Evaporative Liquid Leaks	12.2%	15.8%	12.4%	16.1%
Refueling Vapor	1.5%	21.6%	1.6%	22.1%
Refueling Spillage	28.4%	41.0%	28.9%	41.9%

4.2.2 2020 Fuel Scenarios

For the 2020 scenarios, the profiles used include those from the SPECIATE database along with other assumptions and calculations. The data used by each emission process are described below.

For exhaust emissions, the SPECIATE profiles listed below were used in the evaluation of the 2020 scenarios (where the four-digit profile number is that of the SPECIATE

[31] January and July conditions were used for winter and summer seasons, respectively.

database). Of these, profiles 8757, 8758, and 8754 were based on speciated results from the EPAct test program.

- Profile 8751 was used for exhaust composite emissions (E10 gasoline) for pre-2001 model year light-duty vehicles and all model year heavy-duty vehicles and motorcycles.

- Profile 8757 was used for exhaust composite (E10) for 2001 and newer model year light-duty vehicles.

- Profile 8758 was used for exhaust composite (E15) for 2001 and newer model year light-duty vehicles.

- Profile 8754 was used for exhaust composite (E20) for 2001 and newer model year light-duty vehicles.

For evaporative permeation, the SPECIATE profiles listed below were used in the evaluation of the 2020 scenarios. The profiles for E10 and E20 were developed directly from CRC Project E-65/E-77 results. The profile for E15 was estimated by EPA from interpolation between E10 and E20 results, and was not directly derived from test results on E15.[32]

- Profile 8769, representing evaporative permeation emissions, was used for all evaporative processes with E10 gasoline.

- Profile 8770, representing evaporative permeation emissions, was used for all evaporative processes with E15 gasoline.

- Profile 8773, representing evaporative permeation emissions, was used for all evaporative processes with E20 gasoline.

For evaporative liquid leaks and refueling spillage emissions, the speciation profiles developed were based on existing speciation data for whole gasoline vapor:

- For E10, the mean of two profiles (5493 and 5495) was used;

- For E20, Profile 5494 was used; and

- For E15, a whole gasoline vapor profile was not preexisting and an interpolation between E10 and E20 results was employed.[33]

[32] The details of this interpolation were provided by EPA.
[33] This interpolation followed the method used by EPA to define Profile 8770 (E15 permeation) from E10 and E20 results as described above.

For evaporative vapor and refueling vapor emissions, the speciation profiles developed were based on existing speciation data for whole gasoline vapor:

- For E10, the mean of three profiles (5485, 5487, and 5489) was used;
- For E20, the mean of two profiles (5468 and 5490) was used; and
- For E15, a vapor profile was not preexisting and an interpolation between E10 and E20 results was employed following methods discussed previously.

To incorporate the model-year split in speciation profile assignment for light-duty vehicles, the fraction of emissions occurring from 2001 and newer model year light-duty vehicles was estimated for 2020 using MOVES2010a. The results, shown in Table 4-2, represent national default conditions by season for fleet mix, operation characteristics, and temperature profiles.[34] For example, the first value listed in Table 4-2 signifies that 87.2% of 2020 summer season exhaust composite TOG emissions from passenger cars (PCs) comes from 2001 and newer model years; thereby the remaining 12.8% comes from 2000 and older model year PCs.

Table 4-2
Percent of 2020 TOG Emissions Occurring from 2001 and Newer Model Years
MOVES2010a, National Default Conditions

Emissions Process	PC Summer	PC Winter	LDT Summer	LDT Winter
Exhaust, Composite	87.2%	61.3%	86.1%	53.9%
Evaporative Permeation	83.9%	53.1%	84.0%	53.2%
Evaporative Vapor	81.1%	49.1%	77.8%	43.9%
Evaporative Liquid Leaks	74.7%	50.5%	75.0%	50.9%
Refueling Vapor	67.2%	42.0%	68.3%	42.8%
Refueling Spillage	97.7%	90.7%	97.8%	91.2%

4.3 Results

The speciation data were provided in electronic format. Datasets were developed by scenario, season, and emissions process covering the 3,110 counties in the lower 48 states (those distinguished by FIPS codes in MOVES2010a[24]). The data sets were provided in ASCII file format using comma-delimited records. Each record is defined by eight fields

[34] January and July conditions were used for winter and summer seasons, respectively.

of FIPS, vehicle class, pollutant, CB05 split factor, split factor divisor and species mass fraction.

Four datasets for the 2005 base year scenario were defined for two seasons and two emissions processes separately (exhaust composite and evaporative composite). Each dataset contained between 100,000 and 200,000 records. For each 2020 fuel scenario, 12 datasets were defined for two seasons and seven emissions processes; each dataset contained fewer than 100 records. The number of records in the 2005 datasets is larger due to the county-level variation in the scenarios fuels (absent from the 2020 scenarios); moreover, the number of records in any dataset varies depending on the number of species present (which in turn depends on the emissions process and ethanol blend), as species with a zero split factor were excluded from the final datasets.

For the speciation datasets, there is a single header record in each file. There are eight fields present in each record; these are defined below.

- FIPS: 3110 distinct values from MOVES2010a used for 2005 datasets; "-9" used for 2020 datasets which have no county-level variation
- Vehicle classes: "LDGV", "LDGT1", "LDGT2", "HDGT", "MC"
- Process: "EXHAUST", "EVAPORATIVE", "EVAP PERMEATION", "EVAP LIQUID LEAK", "REFUELING SPILLAGE", "EVAPORATIVE VAPOR", "REFUELING VAPOR"
- Pollutant: "TOG"
- Species: CB05 species name
- Split factor: CB05 split factor as defined in the SMOKE GSPRO file format
- Divisor: split factor divisor as defined in the GSPRO file format
- Mass fraction: species mass fraction as defined in the GSPRO file format

###