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OZONE MODELING PREDICTIONS SENSITIVITY TO SPECIATION OF EXHAUST VOC EMISSIONS

Final Report

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Ozone Modeling Predictions Sensitivity to Speciation of Exhaust VOC Emissions

CRC A-85 Final Report

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EXECUTIVE SUMMARY

Fuel use in motor vehicles results in exhaust and evaporative emissions of volatile organic compounds (VOCs) that participate in atmospheric photochemical reactions and contribute to ambient ozone formation. Such emissions have been regulated through increasingly stricter standards on vehicles in the U.S., such as the recent Federal Tier 3 program, to help attain compliance with national air quality standards for ozone. VOCs released in the exhaust of vehicles have varying effects on ground-level ozone depending on their chemical speciation which in turn depends on the chemical composition of the fuel consumed and vehicle technology, with additional species formed and emitted as products of incomplete combustion. Source-specific speciation profiles, such as the EPA 8757 profile for gasoline exhaust from light-duty vehicles using 10% ethanol, assign emissions of total organic gases (TOG, i.e., VOCs plus non-photochemically reactive compounds such as methane) in the exhaust to model species in air quality models for use in condensed chemical mechanisms.

Vehicle speciation profiles are derived from vehicle testing data that are subject to considerable uncertainty and variability. Because the speciation influences photochemistry, if we examine the sensitivity of predicted ozone concentrations to different speciation profiles, we can gauge the importance of the choice of vehicle organic gas speciation in photochemical air quality modeling.

To that end, we applied the Comprehensive Air Quality Model with Extensions (CAMx) using the Carbon Bond 2005 (CB05) chemical mechanism to estimate the variation in summertime ozone concentrations with three different TOG speciation profiles for on-road gasoline light-duty vehicle (gLDV) exhaust emissions in the U.S. The base speciation profile applied was the aforementioned EPA 8757 profile; the emissions for this profile were obtained from CRC Project A-76-3 and corresponded to low emission vehicle (LEV) III controls and gasoline with 10 ppm sulfur, similar to the Federal Tier 3 standards. The other two TOG profiles were selected from vehicle test measurements conducted by Southwest Research Institute involving fifteen vehicle types and three different fuels in CRC Project E-98. The first of these two profiles represents cold-start Bag 1 emissions for a 10% ethanol fuel identified as Fuel 2 and the second, hot start Bag 3 emissions for the same fuel. The EPA 8757 composite profile used in prior CRC modeling had speciation and reactivity much more similar to the Fuel 2 Bag 1 (F2B1) profile than the Fuel 2 Bag 3 (F2B3) profile. The F2B1 profile has, on average, four times higher ozone reactivity under NOx-rich conditions than the F2B3 profile due to a smaller fraction of methane (14% vs. 57%) and larger fractions of more reactive compounds such as xylene (7% vs. absent), ethene (10% vs. 2%) and terminal olefins (4% vs. 0.5%).



CAMx simulations were conducted for July at 36 km horizontal resolution over the continental U.S. and at 12 km over an eastern U.S. sub-domain, for year 2030 when the Tier 3 standards would have fully phased-in. Natural and anthropogenic emissions from other sources and other modeling inputs were derived from the A-76-3 modeling database and held constant across scenarios.

Because gLDV VOC emissions are expected to constitute a small fraction (approximately 3-4%) of the total U.S. anthropogenic VOC inventory in 2030 following implementation of the Tier 3 rule, the relative contribution of gLDV VOC emissions to total ozone is also expected to be small. Therefore, we also examined the sensitivity of ozone levels due solely to gLDV VOCs to the change in speciation by conducting a scenario with no organic gas emissions from gLDVs, but with other chemical species emissions the same as the three scenarios with three speciation profiles.

When considering ozone due to all sources in July 2030, the spatial differences in the monthly maximum of maximum daily average 8-h (MDA8) ozone between the EPA and F2B3 profiles are small (ranging from -0.7 ppb to 0.04 ppb for the change from EPA to F2B3 profile), with the largest decreases occurring off the New Jersey Coastline (approximately 0.7 ppb or 0.7%). The largest decrease in the monthly mean of MDA8 ozone is 0.3 ppb (or 0.4%, in the Los Angeles basin) on altering the speciation from the EPA profile to F2B3 profile. Changes in MDA8 ozone are further smaller (less than 0.1 ppb at the urban areas and also domain-wide) when comparing results between the cold-start F2B1 profile and the EPA profile. The effect of speciation on ozone is small when considering ozone due to all emission sources because VOC emissions from gLDVs with any of the three speciation profiles considered here represent less than 4% of the total U.S. anthropogenic VOC inventory in 2030 following the Tier 3 rule with 10 ppm gasoline sulfur and more stringent emissions standards for motor vehicles.

Varying exhaust speciation has a large impact on modeled ground-level ozone when assessing the effect on ozone concentrations attributable to just gLDV VOC emissions; the difference in the July mean of daily maximum 8-hour ozone on altering the VOC speciation from the default EPA 8757 profile to the hot-start F2B3 profile is large (57-78%) in some urban areas such as the Los Angeles Basin, Chicago and New York City when considering the fraction of ozone produced solely from gLDV VOCs. This suggests that the choice of vehicle exhaust VOC speciation will be important in some NOx-rich urban areas when vehicle exhaust produces a large fraction of the region's VOC emissions and gLDV VOC emissions are important for ozone formation.

Our analysis of E-98 vehicle testing data indicated several vehicle/fuel combinations where the total mass of individual speciated organic compounds measured was less than the total non-



methane hydrocarbon (NMHC) mass reported, suggesting that some organic compounds were not identified. This finding of low recovery rates is in agreement with the conclusion of May and co-workers (2014) who noted that the chromatographic techniques used to determine the chemical composition of vehicle exhaust may not identify compounds representing up to 25% of the hydrocarbon mass, with the majority being C₇ compounds and larger that may have higher secondary organic aerosol yields in the atmosphere. This is a promising area for future research on the air quality impact of the speciation of organic gases in on-road vehicle tailpipe emissions.



1.0 INTRODUCTION

Volatile organic compounds (VOCs) are a large group of organic chemicals that include any compound of carbon (excluding carbon monoxide, carbon dioxide, carbonic acid, metallic carbides or carbonates, and ammonium carbonate) and that participate in atmospheric photochemical reactions. VOCs are of concern, in part, because they contribute to ambient ground-level ozone (O_3) through interactions with oxides of Nitrogen (NOx) and sunlight. VOCs are released from a variety of sources, both natural (e.g., vegetation and wildfires) and anthropogenic (e.g., fuel combustion in industrial, commercial, institutional and residential sources, other industrial processes, on-road vehicles, off-road vehicles, solvent use and others). In particular, VOCs are emitted from on-road motor vehicles due to fuel use and are present in exhaust emissions and in evaporative emissions such as resting and running losses and fuel tank and engine vapors. The focus of this study is on the effect of the speciation of tailpipe exhaust emissions on ambient O_3 .

The speciation of VOCs released in the exhaust of motor vehicles reflects the chemical composition of the fuel consumed, with additional species formed and emitted as products of incomplete combustion. Photochemical air quality models represent differences in reactivity between individual VOCs to characterize their effect on O₃. Condensed chemical mechanisms (e.g., Carbon Bond 5 (CB05)) use model species to represent the multitude of VOCs present in emissions. Some model species are explicit VOCs whereas others represent classes of VOCs. A "speciation profile" assigns emissions of total organic gas (TOG, which includes all organic gas compounds emitted to the atmosphere including low-reactivity compounds such as methane, ethane, acetone and others) to model species. The speciation profile influences photochemistry and consequently affects the predicted tropospheric O₃ concentrations. The speciation profile uncertainty and/or variability.

The objective of this study is to use a test case to investigate the sensitivity of modeled ambient summertime O₃ concentrations to the variability in the speciation of on-road gasoline light-duty vehicle (gLDV) exhaust emissions in the United States (U.S.) with focus on the eastern U.S. The CRC Atmospheric Impacts Committee co-funded measurements of organic gas speciation in the exhaust emissions of vehicles by the Southwest Research Institute (SwRI) in the CRC Emissions Committee Project E-98 (SwRI, 2013). The speciation profiles in the current study are derived from vehicle test results available from the E-98 study and from the default EPA speciation profile (#8757) applied in a prior CRC study (A-76) conducted by ENVIRON (Vijayaraghavan et al., 2012).



2.0 ANALYSIS OF SPECIATION PROFILE MEASUREMENTS

SwRI provided chemical speciation profiles and criteria pollutant emissions from the E-98 vehicle and fuel test data sets. Vehicle testing was conducted using the LA-92 emissions test cycle. The vehicle testing consisted of the standard Federal Test Procedure (FTP) of a cold start LA-4 driving cycle split into two parts, Bag 1 (cold start) and Bag 2 (hot running), and a hot restart with a repeat of the first part of the LA-4 cycle called Bag 3.

The testing included 15 vehicles and three fuels with two tests. Speciation was reported for a limited number of vehicle/fuel combinations. The data relevant to the current study are captured exhaust methane and speciated VOCs from three different fuels (Fuels 1, 2 and 3) in Bags 1, 2, and 3. Fuel #1 did not contain ethanol and Fuels #2 and #3 contained 10.1% and 15.8% ethanol by volume, respectively. In all, 15 vehicles were tested. Test result validations were not always performed as few replicate speciation measurements of vehicle/fuel combinations were available. Approximately 204 hydrocarbon species, 14 aldehydes and ketones, and 4 alcohols were measured for each profile. ENVIRON calculated 15-vehicle average profiles for each fuel by bag using the sum of the weights (mg/mile) of emission estimates of the vehicles. The final average profiles are provided in Appendix A, Table A-1.

ENVIRON conducted quality assurance (Q/A) tests on the data provided to ensure that individual test results were reasonable and to identify fuel/bag combinations for modeling. In the first QA test, the total speciation recovered was compared with the total reported nonmethane hydrocarbon (NMHC) emissions. If the total speciation did not match well the total hydrocarbon species, then it was determined that the speciation for that test was not representative of the total emissions profile and was either missing important species or had unreasonable compound concentrations. The speciation totals represent NMOG (non-methane organic gas) which includes oxygenated compounds (aldehydes and alcohols) with their full molecular weight unlike NMHC that exclude the carbon and oxygen bound together. Thus, a perfect correlation would result in total NMOG speciation exceeding the NMHC total. We used this test to determine if the speciation recovered a large portion of the hydrocarbon emissions or that the speciation did not greatly exceed the hydrocarbon totals. The NMOG speciation can be corrected to a NMHC estimate, but such a correction does not influence the conclusion of which speciation tests have sufficient recovery rates.

ENVIRON compiled the speciation and composite criteria pollutant data for each vehicle/fuel combination as shown in Appendix A, Table A-2. The recovery fraction was calculated as the total speciation mass divided by the NMHC total mass that provided an alternative measure of a full emissions profile.



Test data were excluded when the recovery rate (fraction) was less than 88% or more than 143%; the next highest recovery rate below 88% was 82% and next lowest rate above 143% was 171%. All but six of the profiles excluded were excluded due to low recovery rates. The Bag 2 and Bag 3 samples had poor recovery rates likely due to low emission rates generating species concentrations below detection limits.

ENVIRON averaged the remaining test results and performed a series of tests to determine if there were any significant outlier chemical species measurement that may affect the average profiles and photochemical reactivity of those profiles. Average profiles were calculated using a sum of the mass emissions of each compound for each fuel and bag combination. The average was calculated using the actual emissions, so that higher emitters contribute more to the average speciation than lower emitters.

An additional Q/A test could exclude outliers at three times the standard deviation, but because of the limited sample sizes, no samples were excluded. The following procedure was used to evaluate tests when individual compounds were found to be outliers:

1. Determined the normalized speciation of each accepted vehicle/fuel/bag sample and estimated the standard deviation and 95% uncertainty for each compound of the accepted samples.

2. Determined outliers using the #1 average +/- #2 uncertainty limits (x3 or x4 the standard deviation) and for components with >2% of the composition. Outliers were identified at the x3 standard deviation test, but just barely, and none at x4 standard deviation.

Discriminating between VOCs on the basis of their contributions to O_3 formation, or reactivities, is not straightforward. Reactivity is not simply a property of the compound itself; it is a property of both the compound and the environment in which the compound is found (EPA, 2005). The reactivity of a single compound varies with VOC-NOx ratios, meteorological conditions, the combination of other VOCs in the atmosphere, and the time interval of interest. Nonetheless, reactivity "scales" or weighting approaches based on the relative reactivity of different VOCs offer a useful tool for examining the relative contribution of individual VOCs to O_3 . In this study, the Maximum Incremental Reactivity (MIR) scale of Carter (2013) was applied; this is the same as the California Air Resources Board (ARB, 2014) MIR factor scale.

The average profiles across 15 vehicles in this study are provided in Appendix A, Table A-1, with the MIR by species and for the overall profile. Table 2.1 provides the number of valid (based on the sufficient and reasonable recovery fraction) test results and the MIR for the average profiles calculated for each fuel/bag combination. The default EPA profile (#8757) used in previous modeling is also provided in Table 2.1. The EPA profile has speciation and reactivity closer to



the Bag 1 profile for all fuels. Bag 1 had the highest reactivity because of a higher fraction of olefins and aromatics, and the lowest methane fraction. Methane was measured and reported separately from the NMOG results and represents a large fraction of the Bag 2 and Bag 3 emissions. The reactivity of Bag 1 for all fuels was considerably higher than for Bags 2 and 3 because methane has a low reactivity and represents most of the TOG speciation in the latter.

Fuel / Bag	Count	Average MIR	Average MIR	Comment
		(g O3 / g TOG)	(g O3 / g VOC)*	
Fuel 1 Bag 1	15	4.08	4.58	8.9% methane
Fuel 1 Bag 2	6	1.68	2.83	36% methane
Fuel 1 Bag 3	3	1.48	2.98	45% methane
Fuel 2 Bag 1**	15	3.85	4.61	14% methane
Fuel 2 Bag 2	2			Insufficient Samples
Fuel 2 Bag 3**	8	0.93	2.41	57% methane
Fuel 3 Bag 1	15	3.64	4.46	16% methane
Fuel 3 Bag 2	1			Only one sample
Fuel 3 Bag 3	4	0.78	2.33	62% methane
EPA Profile 8757		3.76	4.71	17% methane

Table 2.1.	Valid sam	oles with	sufficient	recovery	rates.

* Definition of VOC excludes methane, ethane, and acetone from TOG.¹

** Speciation profiles from Fuel 2 Bag 1 and Fuel 2 Bag 3 were selected for use in air quality modeling

There are additional differences in the speciation depending upon the compound of interest. High reactivity ethylene, propylene, and other olefins are found in considerable amounts, and especially in the Bag 1 speciation. Toluene and other aromatic compounds are also found in significant fractions. For Fuel 3, an unusually large fraction of 2,2,4-trimethylpentane was found compared with the results for the other fuels.

The final averaged speciation profiles for Fuel 2 Bag 1 (cold-start; hereafter referred to as the "F2B1" profile) and Bag 3 (hot-start; hereafter referred to as the "F2B3" profile) were selected for application in air quality modeling. These two averaged profiles were assigned to the corresponding SPECIATE (version 4.3; EPA, 2011b) database ID and used as input to the EPA SPECIATE Tool to create CB05 mechanism profiles for comparison with the EPA profile used in previous work and for air quality modeling.

¹ <u>http://www.epa.gov/ttn/naaqs/ozone/ozonetech/def_voc.htm</u>



2.1 EPA, F2B1, and F2B3 Speciation Profile Comparison

The gLDV organic gas fractional splits are quite similar in the EPA profile and F2B1 cold-start speciation profile (Table 2.2). The largest relative differences between the two profiles among the CB05 species are for internal olefin carbon bonded VOCs (IOLE) and isoprene (ISOP) at 44% and 40%, respectively. However, the fractions of IOLE and ISOP in the EPA profile are very small (approximately 1% and 0.1%, respectively) and hence the difference between profiles is relatively unimportant for these constituents compared to, for example, that for toluene (TOL) which comprises 11% of the total mass in the EPA profile and is higher by 15% in the F2B1 profile. The speciation profile for the F2B3 profile is very different from the EPA profile with most VOC fractions lower by 17% to 95% in the F2B3 profile than the EPA profile while the methane fraction is higher by more 200%, resulting in much lower overall reactivity in the F2B3 profile.

Table 2.2.	Gasoline light-duty vehicle speciation profiles for the EPA (#8757), F2B1, and
F2B3 scena	rios.

	Weight fraction by profile					
Species	EPA 8757	F2B1	F2B3			
ALD2	0.0162	0.0138	0.0008			
ALDX	0.0015	0.0017	0.0042			
CH4	0.1736	0.1441	0.5725			
ETH	0.1005	0.102	0.0191			
ETHA	0.027	0.0218	0.0446			
ETOH	0.0381	0.0427	#N/A			
FORM	0.0148	0.013	0.0036			
IOLE	0.0121	0.0174	0.0093			
ISOP	0.001	0.0014	#N/A			
MEOH	0.0054	0.0041	0.0169			
OLE	0.0416	0.0383	0.0049			
PAR	0.3208	0.3516	0.2656			
TOL	0.1058	0.1218	0.0217			
UNR	0.0445	0.0578	0.0367			
XYL	0.0971	0.0685	#N/A			
Total	1	1.0001	0.9999			



The differences (or lack thereof) between the profiles are clearer when examined in the context of on-road mobile source emissions totals in the 36 km resolution modeling domain (the air quality modeling is discussed in Section 3) and MIR of individual CB05 species (ENVIRON, 2013). The MIR scale provides a method to estimate the potential increases in O₃ due to the changes of a particular VOC sub-species within a complex blend of chemical species. The MIR scale has the limitation that the maximum incremental reactivity is reached only under high-NOx conditions, and the MIR values are dependent on the composition of the entire VOC population. Nonetheless, the MIR offers an approximate method to compare the reactivity of different VOC species here while recognizing this limitation. Compared to the EPA profile, the F2B3 profile results in much smaller emissions of VOCs with moderate to large MIR, such as toluene (TOL), ethene (ETH), terminal olefins (OLE) and xylene (XYL) (reductions of 3295 tons, 2673 tons, 1105 tons, and 2518 tons, respectively) (Table 2.3); these reductions would result in reductions in ozone under NOx-rich conditions. In contrast, the F2B1 profile shows much smaller emissions reductions from the EPA profile because of the similarity in speciation, with emissions increases actually occuring for IOLE, PAR and TOL. In the case of the F2B3 profile, some species like ETH (ethane) and PAR (paraffins) show a large reduction from the EPA profile but have low O₃ reactivity. Some like ISOP (isoprene) have a high MIR but are less important for changes in O₃ production here as they constitute a small fraction of the profile and their emissions changes are very small. Overall, the MIR of the F2B3 "hot-start" exhaust sampling was found to be 75% less reactive than the EPA profile (0.93 g O_3 /g VOC vs. 3.76 g O_3 /g VOC). The O_3 impacts from varying profile use are examined in Section 3.



				Emissions (tons/month)				
CB05 species	Species description	# Carbon Atoms	MIR (mol O ₃ / mol organic compound)	EPA #8757	F2B1	F2B1 - EPA	F2B3	F2B3 - EPA
ALD2	Acetaldehvde	2	4.5	1114	1105	-9	826	-288
ALDX	Propionaldehyde and higher aldehydes	2	6.8	571	572	1	632	61
ETH	Ethene	2	4.4	3487	3474	-13	814	-2673
ETHA	Ethane	2	0.1	684	653	-31	1335	651
ETOH	Ethanol	2	1.0	3612	3635	23	2801	-811
FORM	Formaldehyde	1	4.5	672	674	2	420	-252
IOLE	Internal olefin carbon bond (R- C=C-R)	4	13.1	1211	1238	27	980	-231
ISOP	lsoprene	5	11.6	53	54	1	7	-46
MEOH	Methanol	1	0.4	67	63	-4	243	176
OLE	Terminal olefin carbon bond (R- C=C)	2	8.2	1518	1490	-28	413	-1105
PAR	Paraffin carbon bond (C- C)	1	0.3	33123	33288	165	30384	-2739
TERP	Terpene	10	8.8	52	52	0	52	0
TOL	Toluene	7	2.9	10508	10626	118	7213	-3295
XYL	Xylene	8	14.8	5999	5801	-198	3481	-2518

Table 2.3.On-road mobile emissions from all types of vehicles in the 36 km air qualitymodeling domain in each vehicle speciation profile for selected CB05 species.



On average across the continental U.S. (CONUS), July gLDV VOC emissions are higher by 0.6% in the cold-start F2B1 profile than the EPA profile while the hot-start F2B3 emissions are lower on average by 29% (Table 2.4). Overall, the fraction of total gLDV emissions of all anthropogenic sources is only 4.1% using the EPA profile and 3.9% and 2.9% with the F2B1 and F2B3 profiles, respectively, in summer 2030 with implementation of the Tier 3 Rule (EPA, 2014) (the choice of the 2030 modeling year and the inventories for other emissions are discussed below in Section 3). For comparison, the contributions from area sources and off-road vehicles are approximately 68% and 14%, respectively (Figure 2.1). VOC emissions in Figure 2.1 are not reactivity-weighted and only serve as an illustrative example of the gLDV fractional contribution to the entire VOC inventory. Reactivity-weighted VOCs are not reported here because the change in O₃ does not always follow the change in MIR, especially in NOx-sensitive conditions. For example, note that MIR for the F2B1 samples, on average, is 2% higher than the EPA profile case (see Section 3).

Table 2.4.July 2030 gasoline light-duty vehicle (gLDV) VOC emissions for the ContinentalU.S. (tons/month) using the EPA, F2B1, and F2B3 gLDV speciation profiles and their relativedifferences (%).

Modeling Domain	EPA (#8757)	F2B1	F2B3	Change (%) from EPA profile to F2B1 profile	Change (%) from EPA profile to F2B3 profile
CONUS 36 km	40,512	40,761	28,818	0.6%	-29%
Eastern U.S. 12 km	20,399	20,525	14,478	0.6%	-29%





Figure 2.1. Composition of total CONUS anthropogenic VOC emissions in July 2030 using the EPA, F2B1, and F2B3 gLDV speciation profiles.



3.0 OZONE SENSITIVITY MODELING

Photochemical air quality sensitivity simulations were performed to test the sensitivity of summertime tropospheric O_3 to varying VOC speciation profiles for gLDV exhaust.

3.1 Modeling Domain and Emissions Methods

The air quality simulations were conducted with the Comprehensive Air Quality Model with Extensions (CAMx) (ENVIRON, 2013) using on-road emissions inventories derived using the Motor Vehicle Emission Simulator (MOVES) (EPA, 2010a) and other model inputs as discussed below. We applied version 5.40 of CAMx with the CB05 chemical mechanism and version 2010a of MOVES. Sensitivity simulations were performed for the month of July as O₃ concentrations are generally the highest during the summertime in the eastern U.S. July was the summertime month selected for modeling in the prior CRC A-76-3 study (ENVIRON, 2014) from which some model inputs were obtained as discussed below. We modeled year 2030 following EPA's selection of 2030 as the future year in its Regulatory Impacts Analysis for the Tier 3 motor vehicle emission and fuel standards rulemaking; 70% of the miles travelled in 2030 are from vehicles that meet the fully phased-in Tier 3 standards (EPA, 2014).

The geographic region studied here includes part of the eastern U.S. with focus on four of thirteen urban areas discussed in EPA's PM Risk Assessment analysis (EPA, 2010b). The four areas selected are Atlanta, Detroit, Philadelphia and St. Louis. The CAMx modeling domain extends over the CONUS at 36 km horizontal resolution with an inner nested domain at 12 km grid resolution over part of the eastern U.S. including the four urban areas of interest. The domain and four urban areas are shown in Figure 3.1. The domain has a pressure-based vertical structure with 26 layers with the model top at 145 mb or approximately 14 km above mean sea level.



Figure 3.1. 36 km Continental U.S. and 12 km eastern U.S. air quality modeling domains.

3.1.1 Meteorology

CAMx modeling for the year 2030 scenarios were driven by year 2008 meteorological fields from the Weather Research and Forecast (WRF) model – Advanced Research WRF (ARW) core (Skamarock et al., 2008). WRF output meteorological fields at 12 km horizontal resolution over the CONUS were obtained from the EPA (Gilliam, R., personal communication, 2011) and converted to CAMx input meteorological files for the nested 36 and 12 km grid resolution domains. Data in 34 WRF vertical layers extending up to 50 mb altitude were mapped to 26 layers in CAMx extending up to 145 mb. A limited performance evaluation of the WRF meteorological outputs and CAMx-ready meteorology showed satisfactory performance. The WRF meteorological fields and performance evaluation are described elsewhere (Vijayaraghavan et al., 2012).

3.1.2 On-road Motor Vehicle Emissions

MOVES 2010a was used to prepare on-road emissions inventories in the CONUS for four scenarios:

1. Light-duty gasoline vehicle exhaust emissions using the EPA 8757 speciation profile

2. Light-duty gasoline vehicle exhaust emissions using the cold-start Fuel 2 Bag 1 (F2B1) speciation profile

3. Light-duty gasoline vehicle exhaust emissions using the hot-start Fuel 2 Bag 3 (F2B3) speciation profile

4. Light-duty gasoline vehicle exhaust emissions with no organic gases but with other chemical species the same as the other three scenarios (the purpose of this scenario is to characterize the contribution of LDV VOCs to ambient O_3 by difference with the first scenario)

The on-road emissions for winter and summer from MOVES for all emissions scenarios were speciated to CAMx model species, temporally allocated to hourly emissions, and spatially allocated to grid cells using version 2.7 of the Sparse Matrix Operator Kernel Emissions (SMOKE) model. Average day emissions were adjusted to account for day-of-week and hour-of-day effects based on SCC codes. Emission estimates for total VOC were converted to the CB05 chemical mechanism in CAMx using VOC speciation profiles derived from EPA's SPECIATE database, version 4.3 (EPA, 2011a) and the F2B1 and F2B3 measurements from this study. PM emissions were speciated to CAMx model species, namely primary organic aerosol, primary elemental carbon, primary nitrate, primary sulfate, primary fine other PM, and coarse PM following methods outlined by Baek and DenBleyker (2010). On-road mobile sources generated using MOVES at the county level were allocated to CAMx 36 km and 12 km grid cells using spatial surrogates derived with the Spatial Surrogate Tool.

(http://www.epa.gov/ttn/chief/emch/spatial/spatialsurrogate.html).

3.1.3 Other Emissions

Emissions from other sources were obtained from previous modeling (ENVIRON, 2014). Emissions from anthropogenic area and point sources in the CONUS other than on-road emissions for the 2030 emissions scenarios were compiled from the U.S. EPA 2030 inventory developed for the modeling analysis of the Heavy Duty Vehicle Green House Gas (HDGHG) (EPA, 2011b). The source sectors obtained from the 2030 HDGHG inventory include fugitive dust, agricultural, non-point, electric generating units (EGUs), point sources other than EGUs, aircraft, locomotives, commercial marine vehicles, and non-road sources. EPA estimates for 2020 for anthropogenic area and point emissions for Canada and Mexico (EPA, 2010c) were applied because these sources are not projected to 2030 in the EPA 2030 HDGHG modeling platform. The model simulations applied biogenic emissions of CO, nitric oxide, isoprene and other VOCs, wildfire emissions of CO, NOx, VOCs, SO₂, NH₃ and PM and sea salt emissions of particulate sodium, chloride and sulfate developed previously (Vijayaraghavan et al., 2012) across the CAMx 36 km domain and are held constant across the emission scenarios. All emissions inventories described above are converted to speciated, gridded, temporally varying emissions files suitable for air quality modeling with CAMx in the nested 36/12 km domains and were held constant across the three 2030 scenarios.

3.1.4 Other Model Inputs

Boundary concentrations of O_3 , PM components and precursors, landuse/landcover data and photolysis rates were obtained from prior modeling (Vijayaraghavan et al., 2012) and held constant across the 2030 scenarios.

3.2 Differences in Ozone Impacts between the EPA and F2B1 Light-Duty Vehicle Exhaust Profiles

The spatial differences between the EPA and F2B1 July maximum of daily maximum 8-hour average (MDA8) O₃ are very small (< 0.1 ppb), with the largest decreases of approximately 0.1 ppb (0.1% decrease) occurring off the New Jersey Coastline in the 36 km and 12 km grid resolution modeling domains (Figures 3.2 and 3.3, respectively). The Eastern Seaboard is an area of abundant NOx emissions (Figure 3.4) and NOx-rich (VOC-sensitive) plumes traveling eastward, away from the coast line, may be VOC-limited in terms of O₃ production. A decrease in VOC emissions from the gLDV sector due to the change in speciation profile from EPA to F2B1 profiles is likely the reason for this modeled change in monthly maximum MDA8 O₃. In general, the modeled reductions in July maximum MDA8 O₃ that resulted from switching to the F2B1 from the EPA profile are generally in the most O₃ polluted areas where the baseline MDA8 O₃ concentrations are at or above 80 ppb.

Changes in O_3 at the urban centers of Philadelphia, St. Louis, Detroit, and Atlanta are examined in more detail in Table 3.1; all values tabulated for each urban area are those modeled in the CAMx 12 km grid resolution grid cell in the geographic center of each area reflecting the approximate impact on the local population. Using the EPA speciation profile, Philadelphia had the highest modeled July MDA8 O_3 at 94.3 ppb, while Detroit had the lowest, at 74.9 ppb. The largest percentage difference between the EPA and F2B1 scenarios was -0.02% at St. Louis, a decrease of roughly 0.02 ppb. Despite the larger abundance of gLDVs in these urban areas (Figure 3.5), changes in monthly maximum MDA8 O_3 were found to be less than the domainwide maximum values over the Atlantic Ocean off the New Jersey Coastline (-0.1%) where the regional gLDV VOC emissions are the largest (Figure 3.5).

The change in monthly mean of MDA8 O_3 between the EPA and F2B1 scenarios is less than 0.05 ppb (Figures 3.6 and 3.7), implying that the O_3 impacts from varying the gLDV speciation profiles were more significant, albeit still very small in magnitude, for the monthly maximum O_3 metric than for the monthly average. Moreover, no noticeable increases in either July maximum or monthly mean MDA8 O_3 were found anywhere in the 12 km domain, which is to

be expected due to the small (4%) fraction of gLDV emissions in the anthropogenic VOC inventory in 2030 (Figure 2.1) and because large parts of the eastern U.S. are NO_X-sensitive on average due to large emissions of biogenic isoprene (Chameides et al., 1992; Duncan et al., 2010; Frost et al., 2006), therefore changes in VOC will not usually induce a subsequent change in O₃. Overall, these small differences in the O₃ impacts between the EPA and F2B1 scenarios are due to both the small contribution of gLDV emissions to the entire anthropogenic VOC inventory (3.9% and 4.1%, respectively) (Figure 2.1) and the similarity between the EPA profile and the F2B1 cold-start speciation profile (Table 2.2).

Table 3.1. July 2030 highest 8-hour ozone concentration (ppb) for select eastern U.S. urban centers using the EPA, F2B1, and F2B3 gasoline light-duty vehicle speciation profiles and their relative differences (%).

				Change (%) from EPA	Change (%) from EPA
Urban Center	EPA	F2B1	F2B3	profile to F2B1 profile	profile to F2B3 profile
Philadelphia	94.3	94.3	94.2	-0.01%	-0.09%
St. Louis	86.6	86.6	86.5	-0.02%	-0.14%
Detroit	74.9	74.9	74.8	-0.01%	-0.12%
Atlanta	85.9	85.9	85.8	0.00%	-0.02%





Figure 3.2. Monthly maximum of daily maximum 8-hour ozone for July 2030 scenarios using the EPA, F2B1, and F2B3 gasoline lightduty vehicle speciation profiles, 36 km grid resolution.











Figure 3.4. Total July 2030 CRC-A76 NOx emissions (short tons) from all emission sectors (anthropogenic and biogenic).





Figure 3.5. Total July 2030 gasoline light-duty vehicle (gLDV) exhaust VOC emissions (short tons) using the EPA speciation profile and the percentage (%) of gasoline light-duty vehicle (gLDV) exhaust VOC emissions of the total (anthropogenic plus biogenic) VOC emission.





Figure 3.6. Monthly mean of daily maximum 8-hour ozone for July 2030 scenarios using the EPA, F2B1, and F2B3 gasoline light-duty vehicle speciation profiles, 36 km grid resolution.





Figure 3.7. Monthly mean of daily maximum 8-hour ozone for July 2030 scenarios using the EPA, F2B1, and F2B3 gasoline light-duty vehicle speciation profiles, 12 km grid resolution.



3.3 Differences in Ozone Impacts between the EPA and F2B3 Light-Duty Vehicle Exhaust Profiles

The differences in the July maximum MDA8 O₃ between the EPA and F2B3 scenarios were larger in magnitude than those between the EPA and F2B1 scenarios and range from -0.70 ppb to +0.04 ppb. Like the F2B1 maximum July O_3 impacts, the largest decreases in the 12 km eastern U.S. modeling domain were also adjacent the New Jersey Coastline for the F2B3 scenario, at roughly -0.7 ppb (roughly a 0.7% decrease) and -0.5 ppb (roughly a 0.6 % decrease) in the 36 km CONUS modeling domain over the same area (Figures. 3.2, 3.3). Within the eastern U.S. domain, additional decreases in July maximum MDA8 O_3 above 0.1 ppb were seen over the Chicago metropolitan area, over the southern portion of Lake Michigan, and over the population centers of major eastern U.S. urban areas such as New York city, Pittsburgh, Indianapolis, and Raleigh-Durham. The largest percent difference in maximum July MDA8 O₃ among the four urban centers evaluated in this study under the F2B3 scenario was also over St. Louis (0.14% decrease), with a reduction of roughly 0.1 ppb (Table 3.1). Within the Continental U.S. modeling domain, additional decreases above 0.1 ppb in July maximum MDA8 O₃ occurred near the Florida coastline near Miami-Ft. Lauderdale and in Southern California. The highest relative percentage reductions were roughly 0.6% over Southern California and the area off the New Jersey Coastline, both regions of abundant gLDV emissions (Figure 3.5).

July maximum MDA8 O_3 reductions of 0.02 to 0.10 ppb appear over the urban centers of cities in the 12 km domain (Figure 3.2). Figure 3.4 shows these urban areas are in close proximity to substantial NO_x emissions for an average day in July. In NO_x-saturated (VOC-sensitive) environments, as these areas can sometimes temporarily become under stagnation events, an increase in total VOC, or an increase in the reactivity of VOCs, can enhance O_3 production, and a decrease in total VOC, or a decrease in VOC reactivity, can lead to less O_3 formation.

The differences in the July maximum MDA8 O_3 between the EPA and F2B3 scenarios are slight due to the small (2.9%) fraction of gLDV emissions using the F2B3 profile in the 2030 anthropogenic inventory (Figure 2.1).

Slight enhancements in the July average MDA8 O_3 (+0.01 to 0.10 ppb) appear over some portion of all states in the southeastern U.S. and in areas of central California, with a maximum enhancement over Georgia, South Carolina, and Alabama (Figure 3.2). These generally appear in areas of NO_x-sensitive O₃ production and thus additional VOC concentrations will generally have little effect on O₃ production, assuming NO_x concentrations remain constant. In this sensitivity study, only gLDV organic gas emissions are altered and NO_x emissions are held constant. A series of chemical reaction pathways that alters the NO_x concentrations the over



these regions and generates a very small, but positive, O_3 enhancement is possible as discussed below.

Isoprene can react with OH in the presence of NO to form "isoprene nitrates", a temporary NO_x sink, or could be used to convert NO to NO₂, which can then photolyze and produce O₃ (Lockwood et al., 2010). A potential change in HO_x (HO_x \equiv OH + HO₂) budgets through changes in emissions of gLDV VOC sub-species in the regions of significant biogenic isoprene production, such as the southeastern U.S. and mountainous regions of California, could more readily favor the conversion of NO to NO₂, compared to the alternative of serving as a temporary NO_x sink (e.g. Horowitz et al., 2007).

Compared to the differences between the EPA and F2B1 gLDV speciation profiles, the EPA and F2B3 profiles have considerably different fractional splits between each other. Most notable is the much larger portion of TOG that is present as methane (57.3%) compared to that of the EPA and F2B1 profiles (17.4% and 14.4%, respectively). Methane is essentially non-reactive over short timescales as its lifetime against oxidation by OH is roughly 9 years. Therefore, the methane contribution to O_3 production in VOC-sensitive areas is likely minimal. As shown in Table 2.2, the F2B3 profile has smaller amounts of xylene, ethene, and olefins than the EPA profile. The MIR of xylene, ethene, and olefins are large (14.8, 4.4, and 8.2 mol O_3 /mol VOC, respectively), while the MIR of methane is several orders of magnitude less.

The replacement of more reactive VOC species (such as xylene, ethene, and olefins) with less reactive methane is likely a major reason for the peak decreases in the July maximum MDA8 O_3 between the F2B3 and the EPA profile, especially in polluted areas where NO_x is high (i.e., where maximum incremental reactivity can be achieved). It should be noted that while the overall MIR of the F2B1 profile was measured to be greater than the EPA profile, the simulation using the latter, less reactive gLDV profile produced slightly greater O_3 than the simulation that used the former, more reactive profile. Although this may seem counter-intuitive, the MIR scale is not always a truthful measure of how much O_3 will be produced with in a chemical environment. The MIR is a theoretical limit under NO_x–rich conditions; if these conditions are not present, the MIR may not necessarily be an accurate metric from which to broadly forecast O_3 production.

A feature of both F2B1 and F2B3 scenarios is the prominence of monthly maximum MDA8 O_3 impacts over water, specifically, the Great Lakes, the Atlantic Ocean off the Coast of the New Jersey and Miami, the Chesapeake Bay, and the Pacific Ocean off the Coast of California (Figures 3.2, 3.3). Over water, the temperature profile can sometimes be cooler than that of the surrounding land. In the summertime when most higher O_3 events occur, this is particularly



true of the surface water temperature of the Great Lakes, the Pacific Ocean off the coast of Southern California and the Chesapeake Bay (Goldberg et al., 2014). Daytime mixing heights in these areas are can be lower than those over the adjacent land. This can locally trap pollutants (NOx and VOCs transported from over land) in a smaller volume and lead to higher concentrations. Additionally, O_3 dry deposition rates are slower over water than over vegetated land areas (Gallagher et al., 2001). Ozone concentrations in these areas can be reduced if VOC emissions decline or if the profile is less reactive (i.e., smaller MIR); both of these are the case for the F2B3 profile.

When considering ozone due to just gLDV VOCs, isolated parts of the country (in the Los Angeles basin, the San Francisco Bay area, Houston, Tampa, Miami, Chicago, Detroit and part of New York city) exhibit a much stronger effect on O₃ concentrations from the change in speciation from EPA #8757 to F2B3 profiles (Figures 3.8 and 3.9). The urban areas listed above also generally correspond to areas with a relatively large reduction in gLDV VOC emissions from the EPA profile to F2B3 profile scenarios (Figure 3.10). While the gLDV VOC contribution to ozone itself is low (<0.6 ppb of monthly mean MDA8 O₃ across the country) (Figure 3.8), the relative reduction in ozone due to gLDV VOC emissions ranges from 57% (in the Los Angeles basin) to 78% (in New York City) on altering the VOC speciation from the EPA profile to the F2B3 profile in these urban areas (Figure 3.9). The range in reduction of 57% to 78% is comparable to the 75% reduction in average MIR from the EPA to F2B3 profiles (Table 2.1), suggesting that these are VOC-sensitive areas where the MIR provides an indirect approximate measure of the effect of speciation on the reduction in ozone due to just gLDV VOC emissions.





Figure 3.8. Monthly mean of daily maximum 8-hour ozone in July 2030: Ozone due to VOCs from gasoline light-duty vehicles only (top) and the relative change in such ozone on altering the VOC speciation from the EPA profile to the F2B3 profile (bottom), 36 km grid resolution.





Figure 3.9. Monthly mean of daily maximum 8-hour ozone in July 2030: Ozone due to VOCs from gasoline light-duty vehicles only (top) and the relative change in such ozone on altering the VOC speciation from the EPA profile to the F2B3 profile (bottom), 12 km grid resolution.







Figure 3.10. Change in total VOC emissions from gasoline light-duty vehicles on altering the VOC speciation from the EPA 8757 profile to the F2B3 profile.



4.0 CONCLUSION AND IMPLICATIONS

Emissions standards for organic gases from LDVs have become increasingly stringent in the evolution from the Tier 0 to Tier 3 standards. Thus, while considerable differences exist between the composite EPA 8757 profile and the hot-start F2B3 speciation profile modeled in this project, the change in speciation has a very small effect on total O₃ due to all sources because of the small fraction (<4%) of gLDV VOCs in the total U.S. anthropogenic VOC inventory in 2030 and because several parts of the U.S., especially the eastern U.S., are NOx-limited due to large biogenic emissions. Therefore, the relative change in MDA8 O₃ in July 2030 on altering the speciation is also small, with a maximum reduction of 0.7 ppb for the monthly maximum of MDA8 O₃ (off the coast of New Jersey/New York) and 0.3 ppb for the monthly mean of MDA8 O₃ (in the Los Angeles basin). The larger differences between the F2B3 and the EPA profile than between the F2B1 and EPA profiles are attributable to the greater fraction of methane within the F2B3 profile and the reduced fraction or absence of more reactive VOCs such as xylene and ethene.

It is important to note, however, that the change in ozone due to the speciation change from the default EPA 8757 profile to the hot-start F2B3 profile is large (57-78%) in some NOx-rich urban areas when considered as a fraction of the July mean MDA8 O_3 produced from just gLDV emissions. This suggests that the choice of gLDV speciation could be important in areas where gLDV emissions are a limiting precursor for ozone production.

One potential issue with using a detailed speciation profile with separate start and running profiles is that it may obscure further evaluation of the effect that emission inventory uncertainty has on air quality. For example, a recurring concern about the light-duty vehicle exhaust emission estimates is that high emitters have been underestimated. A high emitter is more likely to have a failing catalyst than a normal emitter. Because both start and running high emitter exhaust emissions would have a speciation profile more similar to start exhaust, inventory modelers may ignore the need for an accurate speciation for running exhaust emissions consisting of a mix of high and normal emitting vehicles where high emitters would produce more reactive running emissions.

May and co-workers (2014) have noted that the chromatographic techniques used to determine the chemical composition (or speciation) of vehicle exhaust may not identify compounds representing up to 25% of the hydrocarbon mass that may have higher secondary organic aerosol (SOA) yields in the atmosphere. In this work, it was noted that recovery rates for the speciation results were typically below 100% indicating a fraction of unidentified compounds. Also, May et al. reported that unidentified compounds represent about 25% of



hydrocarbon mass. May went further and posited that these unidentified compounds are likely a combination of oxidized compounds that do not elute through the gas chromatograph (GC) column or are found by the techniques used to measure aldehydes and alcohols, indistinguishable isomers that cannot be separated in the GC column, or lower-volatility organic compounds that do not elute in the GC column yet are quantified by the THC flame ionization detector. Future work should consider studies to develop better methods to identify a wider range of vehicle exhaust VOC compounds, and to verify that unidentified compounds do not comprise an important fraction of vehicle exhaust.



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APPENDIX A

Exhaust Profile Measurements



Appendix A. Exhaust Profile Measurements

Table A-1. Average profiles and Maximum Incremental Reactivity (MIR) for each compound.

		Fuel 1	Fuel 1	Fuel 1	Fuel 2	Fuel 2	Fuel 3	Fuel 3	EPA Profile
Compound	MIR	Bag 1	Bag 2	Bag 3	Bag 1	Bag 3	Bag 1	Bag 3	8757
MIR Average		4.08	1.68	1.48	3.85	0.93	3.64	0.78	3.76
METHANE	0.0144	8.86%	35.83%	45.29%	14.41%	57.25%	15.46%	61.75%	17.36%
ETHANE	0.28	2.00%	5.05%	5.45%	2.18%	4.46%	2.75%	5.49%	2.70%
ETHYLENE	9.00	8.64%	3.91%	4.47%	10.20%	1.91%	8.45%	1.68%	10.05%
PROPANE	0.49	0.11%	0.74%	0.93%	0.10%	0.05%	0.10%	0.18%	0.15%
PROPYLENE	11.66	5.10%	2.22%	1.80%	4.56%	0.50%	5.18%	0.77%	3.99%
ACETYLENE	0.95	1.33%	0.35%	0.37%	1.94%	0.19%	1.49%	0.12%	1.65%
PROPADIENE	8.45	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
BUTANE	1.15	2.16%	3.42%	3.04%	1.85%	3.05%	2.60%	2.18%	3.55%
TRANS-2-BUTENE	15.16	0.76%	0.00%	0.22%	0.77%	0.07%	0.60%	0.00%	0.36%
1-BUTENE	9.73	0.44%	0.00%	0.00%	0.42%	0.14%	0.38%	0.00%	0.68%
2-METHYLPROPENE (ISOBUTYLENE)	6.29	3.59%	1.97%	1.55%	3.02%	0.54%	4.70%	0.77%	1.92%
2,2-DIMETHYLPROPANE (NEOPENTANE)	0.67	1.89%	1.39%	1.19%	2.12%	1.48%	0.14%	0.00%	-
PROPYNE	6.72	0.08%	0.00%	0.00%	0.00%	0.00%	0.11%	0.00%	-
1,3-BUTADIENE	12.61	0.51%	0.00%	0.00%	0.46%	0.00%	0.42%	0.00%	0.89%
2-METHYLPROPANE (ISOBUTANE)	1.23	0.21%	0.09%	0.00%	0.35%	0.00%	0.13%	0.10%	-
1-BUTYNE	6.11	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-2-BUTENE	14.24	0.43%	0.00%	0.00%	0.52%	0.00%	0.37%	0.00%	0.29%
3-METHYL-1-BUTENE	6.99	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2-METHYLBUTANE (ISOPENTANE)	1.45	4.35%	7.20%	4.12%	3.31%	4.97%	2.55%	2.06%	0.67%
2-BUTYNE	16.32	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1-PENTENE	7.21	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2-METHYL-1-BUTENE	6.40	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
PENTANE	1.31	2.28%	2.77%	2.20%	1.90%	1.32%	1.57%	1.66%	0.12%
UNIDENTIFIED C5 OLEFINS	3.95	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2-METHYL-1,3-BUTADIENE	10.61	0.17%	0.00%	0.00%	0.14%	0.00%	0.16%	0.00%	0.10%
TRANS-2-PENTENE	10.56	0.07%	0.00%	0.00%	0.06%	0.19%	0.06%	0.00%	0.05%
3,3-DIMETHYL-1-BUTENE	5.82	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-2-PENTENE	10.38	0.03%	0.00%	0.00%	0.03%	0.00%	0.02%	0.00%	0.22%
2-METHYL-2-BUTENE	14.08	0.29%	0.00%	0.00%	0.26%	0.00%	0.24%	0.00%	-
CYCLOPENTADIENE	6.98	0.20%	0.00%	0.00%	0.21%	0.00%	0.14%	0.00%	0.13%
2,2-DIMETHYLBUTANE	1.17	0.76%	1.00%	0.96%	0.95%	1.90%	0.08%	0.00%	0.02%
CYCLOPENTENE	6.77	0.15%	0.00%	0.00%	0.20%	0.89%	0.08%	0.00%	0.06%
4-METHYL-1-PENTENE	5.68	0.51%	0.55%	1.03%	0.08%	0.00%	0.04%	0.00%	0.05%
3-METHYL-1-PENTENE	6.14	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CYCLOPENTANE	2.39	1.21%	0.50%	0.14%	3.61%	0.00%	0.09%	0.00%	-
2,3-DIMETHYLBUTANE	0.97	0.52%	0.58%	0.51%	0.38%	0.27%	0.43%	0.11%	0.27%
4-METHYL-CIS-2-PENTENE	8.12	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2-METHYLPENTANE	1.50	0.98%	0.98%	0.82%	0.99%	1.20%	0.66%	0.47%	1.01%
4-METHYL-TRANS-2-PENTENE	8.12	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.02%
3-METHYLPENTANE	1.80	0.56%	0.58%	0.42%	0.78%	0.60%	0.38%	0.11%	1.14%
2-METHYL-1-PENTENE	5.26	0.02%	0.00%	0.00%	0.01%	0.16%	0.01%	0.00%	0.54%
1-HEXENE	5.49	0.02%	0.00%	0.00%	0.01%	0.16%	0.01%	0.00%	0.54%
HEXANE		0.98%	0.83%	0.75%	1.85%	1.29%	0.66%	0.32%	2.91%
UNIDENTIFIED C6		0.02%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.02%
TRANS-3-HEXENE	7.57	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-3-HEXENE	7.61	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.03%
DI-ISOPROPYL ETHER	3.52	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-2-HEXENE	8.62	0.01%	0.00%	0.00%	0.01%	0.00%	0.01%	0.00%	0.03%
3-METHYL-TRANS-2-PENTENE	13.17	0.02%	0.00%	0.00%	0.02%	0.00%	0.01%	0.00%	0.02%



		Fuel 1	Fuel 1	Fuel 1	Fuel 2	Fuel 2	Fuel 3	Fuel 3	EPA Profile
Compound	MIR	Bag 1	Bag 2	Bag 3	Bag 1	Bag 3	Bag 1	Bag 3	8757
2-METHYL-2-PENTENE	11.00	0.02%	0.00%	0.00%	0.03%	0.00%	0.03%	0.00%	-
3-METHYLCYCLOPENTENE	5.10	0.01%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	-
CIS-2-HEXENE	8.31	0.01%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	-
3-METHYL-CIS-2-PENTENE	13.17	0.02%	0.14%	0.00%	0.01%	0.00%	0.02%	0.00%	-
2,2-DIMETHYLPENTANE, NOTE A	1.12	0.27%	0.11%	0.13%	0.40%	0.50%	0.17%	0.05%	0.40%
METHYLCYCLOPENTANE, NOTE A	2.19	0.27%	0.10%	0.13%	0.40%	0.50%	0.17%	0.05%	0.39%
2,4-DIMETHYLPENTANE	1.55	0.38%	0.18%	0.36%	0.35%	0.17%	0.33%	0.00%	0.27%
2,2,3-TRIMETHYLBUTANE	1.11	0.04%	0.17%	0.00%	0.05%	0.08%	0.04%	0.00%	0.02%
3,4-DIMETHYL-1-PENTENE	4.84	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1-METHYLCYCLOPENTENE	12.49	0.02%	0.00%	0.00%	0.02%	0.00%	0.03%	0.00%	0.00%
BENZENE	0.72	4.63%	5.93%	2.78%	4.21%	2.90%	3.49%	2.58%	3.79%
3-METHYL-1-HEXENE	4.41	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
3,3-DIMETHYLPENTANE	1.20	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CYCLOHEXANE	1.25	0.43%	0.33%	0.00%	0.73%	0.10%	0.24%	0.15%	5.62%
2-METHYLHEXANE	1.19	0.55%	0.64%	0.58%	0.62%	0.70%	0.45%	0.41%	-
2,3-DIMETHYLPENTANE	1.34	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.55%
1,1-DIMETHYLCYCLOPENTANE	1.08	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	0.01%
TERT-AMYL METHYL ETHER	1.69	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CYCLOHEXENE	5.00	0.02%	0.00%	0.00%	0.01%	0.00%	0.01%	0.00%	0.21%
3-METHYLHEXANE	1.61	0.27%	0.23%	0.26%	0.34%	0.06%	0.20%	0.00%	0.25%
CIS-1,3-DIMETHYLCYCLOPENTANE	1.94	0.07%	0.00%	0.00%	0.08%	0.00%	0.04%	0.00%	0.02%
3-ETHYLPENTANE	1.90	0.00%	0.00%	0.00%	0.08%	0.00%	0.00%	0.00%	0.02%
TRANS-1,2-DIMETHYLCYCLOPENTANE	1.99	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%
TRANS-1,3-DIMETHYLCYCLOPENTANE	1.94	0.06%	0.00%	0.00%	0.07%	0.00%	0.03%	0.00%	-
1-HEPTENE	4.43	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,2,4-TRIMETHYLPENTANE	1.26	3.28%	3.97%	3.58%	2.28%	2.22%	9.48%	9.75%	1.23%
2-METHYL-1-HEXENE	5.10	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-3-HEPTENE	6.32	0.04%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
HEPTANE	1.07	1.57%	1.38%	1.30%	0.38%	0.12%	0.37%	0.13%	0.29%
CIS-3-HEPTENE	6.33	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
UNIDENTIFIED C7	1.48	0.02%	0.00%	0.42%	0.02%	0.16%	0.05%	0.00%	-
2-METHYL-2-HEXENE	9.47	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	_
3-METHYL-TRANS-3-HEXENE	9.72	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
ΤΡΔΝΣ-2-ΗΕΡΤΕΝΕ	7 14	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
3-FTHVI-CIS-2-PENTENE	9.75	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
	3 3/	1.02%	0.00%	0.00%	0.00%	0.00%	1.04%	0.00%	0 33%
2 3-DIMETHYL 2-DENITENE	9.74	0.00%	0.13%	0.00%	0.01%	0.23%	0.00%	0.00%	0.5570
	7 16	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
	1 70	0.00%	0.00%	0.00%	0.58%	0.00%	0.00%	0.00%	0.48%
	1 00	0.00%	0.40%	0.40%	0.00%	0.40%	0.40%	0.27%	0.40/0
2 2-DIMETHYLHEXANE	1.55	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
	1.02	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
	6.29	0.04%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	0 13%
	1 22	0.30%	0.00%	0.00%	0.32%	0.00%	0.53%	0.00%	0.13%
	1.22	0.43%	0.00%	0.00%	0.33%	0.00%	0.00%	0.00%	0.1876
	2.01	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
	2.01	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	- 0.19%
1 TRANS 2 CIS A TRIMETHYLCYCLORENTANE	1.75	0.37%	0.32%	0.37%	0.29%	0.00%	0.93%	0.00%	0.18%
	1.33	0.02%	0.00%	0.00%	0.01%	0.00%	0.01%	0.00%	-
	1.24	0.00%	0.00%	0.17%	0.00%	0.00%	0.00%	0.00%	-
	1.03	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.250/
	1.03	1.00%	0.03%	0.90%	0.72%	0.57%	1.01%	1 6 20/	0.35%
	1.02	16 110/	2.07%	1.52%	10.444	0.91%	0.85%	1.02%	0.30%
	4.00	0.20%	7.51%	0.00%	0.120/	2.06%	0.10%	2.94%	7.44%
	1.19	0.30%	0.00%	0.00%	0.13%	0.00%	0.13%	0.00%	0.00%



		Fuel 1	Fuel 1	Fuel 1	Fuel 2	Fuel 2	Fuel 3	Fuel 3	EPA Profile
Compound	MIR	Bag 1	Bag 2	Bag 3	Bag 1	Bag 3	Bag 1	Bag 3	8757
1,1,2-TRIMETHYLCYCLOPENTANE	1.12	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2-METHYLHEPTANE	1.07	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.13%
3,4-DIMETHYLHEXANE, NOTE B	1.51	0.03%	0.00%	0.00%	0.03%	0.00%	0.01%	0.00%	-
4-METHYLHEPTANE	1.25	0.12%	0.12%	0.00%	0.10%	0.00%	0.11%	0.00%	0.00%
3-METHYLHEPTANE	1.24	0.09%	0.00%	0.00%	0.03%	0.00%	0.07%	0.00%	0.10%
1-CIS,2-TRANS,3-TRIMETHYLCYCLOPENTANE	1.63	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.07%
CIS-1,3-DIMETHYLCYCLOHEXANE	1.52	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-1,4-DIMETHYLCYCLOHEXANE	1.62	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.02%
3-ETHYLHEXANE	0.90	0.03%	0.00%	0.00%	0.03%	0.00%	0.00%	0.00%	0.03%
2,2,5-TRIMETHYLHEXANE	1.13	0.46%	0.07%	0.00%	0.36%	0.00%	0.40%	0.00%	0.18%
TRANS-1-METHYL-3-ETHYLCYCLOPENTANE	1.36	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-1-METHYL-3-ETHYLCYCLOPENTANE	1.36	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1,1-DIMETHYLCYCLOHEXANE	1.22	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-1-METHYL-2-ETHYLCYCLOPENTANE	1.36	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1-METHYL-1-ETHYL-CYCLOPENTANE	1.36	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,4,4-TRIMETHYLHEXANE	1.34	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,2,4-TRIMETHYLHEXANE	1.26	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-1,2-DIMETHYLCYCLOHEXANE	1.36	0.02%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.02%
1-OCTENE	3.25	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-4-OCTENE	4.81	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
OCTANE	0.90	0.15%	0.00%	0.00%	0.08%	0.00%	0.17%	0.00%	0.24%
UNIDENTIFIED C8	1.27	0.02%	0.00%	0.00%	0.04%	0.00%	0.01%	0.00%	-
TRANS-2-OCTENE	6.00	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
TRANS-1.3-DIMETHYLCYCLOHEXANE. NOTE C	1.52	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-2-OCTENE	6.00	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
ISOPROPYLCYCLOPENTANE	1.47	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,2-DIMETHYLHEPTANE	1.00	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,3,5-TRIMETHYLHEXANE	1.22	0.06%	0.00%	0.00%	0.03%	0.00%	0.05%	0.00%	-
CIS-1-METHYL-2-ETHYLCYCLOPENTANE	1.47	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,4-DIMETHYLHEPTANE	1.38	0.02%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.02%
4,4-DIMETHYLHEPTANE	1.27	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-1,2-DIMETHYLCYCLOHEXANE	1.47	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.03%
ETHYLCYCLOHEXANE	1.47	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.08%
2,6-DIMETHYLHEPTANE, NOTE D	1.04	0.04%	0.00%	0.00%	0.02%	0.00%	0.05%	0.00%	-
1,1,3-TRIMETHYLCYCLOHEXANE	1.19	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,5-DIMETHYLHEPTANE, NOTE E	1.35	0.02%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	0.02%
3.3-DIMETHYLHEPTANE	1.13	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
3.5-DIMETHYLHEPTANE. NOTE E	1.56	0.02%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	0.02%
ETHYLBENZENE	3.04	1.15%	0.00%	0.00%	1.39%	0.00%	0.80%	0.00%	1.66%
2.3.4-TRIMETHYLHEXANE	1.22	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2,3-DIMETHYLHEPTANE	1.09	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
m-& p-XYLENE	9.75	1.49%	0.00%	0.00%	3.95%	0.00%	1.19%	0.00%	4.35%
4-METHYLOCTANE	0.95	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
3,4-DIMETHYLHEPTANE	1.24	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
4-ETHYLHEPTANE	1.22	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
2-METHYLOCTANE	0.83	0.04%	0.00%	0.00%	0.00%	0.00%	0.05%	0.00%	0.09%
3-METHYLOCTANE	0.99	0.02%	0.00%	0.00%	0.00%	0.00%	0.04%	0.00%	0.04%
STYRENE	1.73	0.35%	0.00%	0.00%	0.19%	0.00%	0.22%	0.00%	0.08%
o-XYLENE		1.03%	0.00%	0.00%	1.24%	0.00%	0.77%	0.00%	1.70%
1-NONENE	2.60	0.04%	0.00%	0.00%	0.01%	0.00%	0.07%	0.00%	0.02%
TRANS-3-NONENE	4.54	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
CIS-3-NONENE	4.54	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
NONANE	0.78	0.09%	0.57%	0.00%	0.02%	0.00%	0.09%	0.00%	0.14%
TRANS-2-NONENE	4.54	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-



Compound MIR Bag 1 Bag 2 Bag 3 Bag 3 <t< th=""><th></th><th></th><th>Fuel 1</th><th>Fuel 1</th><th>Fuel 1</th><th>Fuel 2</th><th>Fuel 2</th><th>Fuel 3</th><th>Fuel 3</th><th>EPA Profile</th></t<>			Fuel 1	Fuel 1	Fuel 1	Fuel 2	Fuel 2	Fuel 3	Fuel 3	EPA Profile
SOPROPUBENZENN (CUMENE) 2.52 0.00%	Compound	MIR	Bag 1	Bag 2	Bag 3	Bag 1	Bag 3	Bag 1	Bag 3	8757
2.2-DIMETHYLOCTANE 0.83 0.00%	ISOPROPYLBENZENE (CUMENE)	2.52	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	0.12%
2.4-DIMETHYLOCTANE 1.02 0.01% 0.00% <td>2,2-DIMETHYLOCTANE</td> <td>0.83</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.15%</td>	2,2-DIMETHYLOCTANE	0.83	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.15%
0-PROPULENZENE 2.03 0.03% 0.00%	2,4-DIMETHYLOCTANE	1.03	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.10%
1-METHYL-3-TTHYLBENZENE 7.39 1.26% 0.00% 0.39% 0.00% 0.37% 0.00% 0.61% 1.3,5-TRIMETHYLBENZENE 11.76 0.92% 0.00% 0.39% 0.00% 0.65% 0.00% 0.65% 0.00% 0.65% 0.00% 0.65% 0.00% 0.65% 0.00% 0.65% 0.00% 0.65% 0.00% 0.00% 0.65% 0.00%	n-PROPYLBENZENE	2.03	0.31%	0.00%	0.00%	0.08%	0.00%	0.19%	0.00%	0.40%
1-METHYL-A-TTYUBENZENE 4.44 0.41% 0.00% 0.01% 0.37% 0.00% 0.68% 0.00% 0.68% 0.00% 0.68% 0.00% 0.68% 0.00% 0.68% 0.00% 0.68% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.05% 0.61% 0.00% 0.05% 0.00%<	1-METHYL-3-ETHYLBENZENE	7.39	1.26%	0.00%	0.00%	0.39%	0.00%	0.95%	0.00%	1.35%
1.3.5. TRINETHYLEBNZENE 11.76 0.92% 0.00% 0.63% 0.00% 0.63% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.54% 0.00% 0.	1-METHYL-4-ETHYLBENZENE	4.44	0.41%	0.00%	0.00%	0.14%	0.00%	0.37%	0.00%	0.61%
1-METHYL-2-ETHYLBENZENE 5.59 0.65% 0.00% 0.613% 0.00% 1.47% 1.2.4-TRIMETHYLBENZENE 8.87 2.51% 0.00%	1,3,5-TRIMETHYLBENZENE	11.76	0.92%	0.00%	0.00%	0.39%	0.00%	0.68%	0.00%	0.62%
12.4-TRINETHVLENZENE 8.87 2.51% 0.52% 0.00%<	1-METHYL-2-ETHYLBENZENE	5.59	0.69%	0.06%	0.00%	0.61%	0.00%	0.54%	0.00%	0.51%
TRAT-BUTYLEENZENE 1.95 0.00% <td>1,2,4-TRIMETHYLBENZENE</td> <td>8.87</td> <td>2.51%</td> <td>0.52%</td> <td>0.00%</td> <td>0.32%</td> <td>0.00%</td> <td>1.47%</td> <td>0.00%</td> <td>1.14%</td>	1,2,4-TRIMETHYLBENZENE	8.87	2.51%	0.52%	0.00%	0.32%	0.00%	1.47%	0.00%	1.14%
1-DECENE 2.17 0.00% <	TERT-BUTYLBENZENE	1.95	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
DECAME, NOTE F 0.68 0.02% 0.21% 0.00% 0.02% 0.00%	1-DECENE	2.17	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
SOBUTYLEENZENE, NOTE F 5.76 0.02% 0.00% 0.02% 0.02% 0.00%<	DECANE, NOTE F	0.68	0.02%	0.21%	0.00%	0.27%	0.16%	0.02%	0.00%	0.08%
1,3,DIMETHYL-S-ETHYLBENZENE 10.08 0.00% <t< td=""><td>ISOBUTYLBENZENE, NOTE F</td><td>5.76</td><td>0.02%</td><td>0.20%</td><td>0.00%</td><td>0.25%</td><td>0.15%</td><td>0.02%</td><td>0.00%</td><td>0.04%</td></t<>	ISOBUTYLBENZENE, NOTE F	5.76	0.02%	0.20%	0.00%	0.25%	0.15%	0.02%	0.00%	0.04%
METHYLPROPYLBENZENE (sec butylbenzene) 2.36 0.01% 0.00%	1,3,-DIMETHYL-5-ETHYLBENZENE	10.08	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1-METHYL-3-ISOPROPYLBENZENE 7.10 0.00% 0	METHYLPROPYLBENZENE (sec butylbenzene)	2.36	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1,2,3-TRIMETHYLBENZENE 11.97 0.36% 0.00% 0.0	1-METHYL-3-ISOPROPYLBENZENE	7.10	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.06%
1-METHYL-4-ISOPROPYLBENZENE 4.44 0.00% 0	1,2,3-TRIMETHYLBENZENE	11.97	0.36%	0.00%	0.00%	0.00%	0.00%	0.13%	0.00%	0.20%
INDAN 3.32 0.00%	1-METHYL-4-ISOPROPYLBENZENE	4.44	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.02%
1-METHYL-2-ISOPROPYLBENZENE 5.49 0.04% 0.00% 0	INDAN	3.32	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.11%
1.3-DIETHYLBENZENE 7.10 0.00% <td>1-METHYL-2-ISOPROPYLBENZENE</td> <td>5.49</td> <td>0.04%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.02%</td> <td>0.00%</td> <td>0.02%</td>	1-METHYL-2-ISOPROPYLBENZENE	5.49	0.04%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	0.02%
1.4-DIETHYLBENZENE 4.43 0.04% 0.00% <td></td> <td>7.10</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.28%</td>		7.10	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.28%
1.METHYL-3-N-PROPYLBENZENE 7.10 0.06% 0.00%	1.4-DIFTHYI BENZENE	4.43	0.04%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.07%
1.METHYL-4-N-PROPYLBENZENE, NOTE G 4.43 0.00%	1-METHYL-3-N-PROPYLBENZENE	7 10	0.06%	0.00%	0.00%	0.00%	0.00%	0.03%	0.00%	-
1,2 DIETHYLBENZENE 5.49 0.02% 0.00% <td>1-METHYL-4-N-PROPYLBENZENE, NOTE G</td> <td>4.43</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>_</td>	1-METHYL-4-N-PROPYLBENZENE, NOTE G	4.43	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	_
IMETHYL-2-N-PROPYLBENZENE 5.49 0.00% 0.0	1.2 DIFTHYI BENZENE	5.49	0.02%	0.00%	0.00%	0.01%	0.00%	0.08%	0.00%	0.05%
1.4-DIMETHYL-2-ETHYLBENZENE 7.55 0.11% 0.00% <td< td=""><td>1-METHYI -2-N-PROPYI BENZENE</td><td>5.49</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.01%</td><td>0.00%</td><td>-</td></td<>	1-METHYI -2-N-PROPYI BENZENE	5.49	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	-
1.3-DIMETHYL-4-ETHYLBENZENE 7.55 0.02% 0.00% <td< td=""><td>1.4-DIMETHYI -2-ETHYI BENZENE</td><td>7.55</td><td>0.11%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.04%</td><td>0.00%</td><td>-</td></td<>	1.4-DIMETHYI -2-ETHYI BENZENE	7.55	0.11%	0.00%	0.00%	0.00%	0.00%	0.04%	0.00%	-
1.2-DIMETHYL-4-ETHYLBENZENE 7.55 0.01% 0.00% <td< td=""><td>1.3-DIMETHYI -4-ETHYI BENZENE</td><td>7.55</td><td>0.02%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.06%</td><td>0.00%</td><td>-</td></td<>	1.3-DIMETHYI -4-ETHYI BENZENE	7.55	0.02%	0.00%	0.00%	0.00%	0.00%	0.06%	0.00%	-
1,3-DIMETHYL-2-ETHYLBENZENE 10.15 0.00% <t< td=""><td>1.2-DIMETHYL-4-ETHYLBENZENE</td><td>7.55</td><td>0.01%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.02%</td><td>0.00%</td><td>-</td></t<>	1.2-DIMETHYL-4-ETHYLBENZENE	7.55	0.01%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	-
DUNDECANE DOING DOING <thdoing< th=""> DOING DOING</thdoing<>	1.3-DIMETHYI -2-ETHYI BENZENE	10.15	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	-
1,2-DIMETHYL-3-ETHYLBENZENE 10.15 0.00% <t< td=""><td></td><td>0.61</td><td>0.13%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.05%</td><td>0.00%</td><td>0.01%</td></t<>		0.61	0.13%	0.00%	0.00%	0.00%	0.00%	0.05%	0.00%	0.01%
1,2,4,5-TETRAMETHYLBENZENE 9.26 0.12% 0.00%	1.2-DIMETHYL-3-ETHYLBENZENE	10.15	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0101/0
2)	1 2 4 5-TETRAMETHYI BENZENE	9.26	0.12%	0.00%	0.00%	0.00%	0.00%	0.04%	0.00%	0 12%
3.4 DIMETHYLCUMENE 8.90 0.00% <td>2-METHYLBUTYLBENZENE (sec AMYLBENZENE)</td> <td>4.73</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>-</td>	2-METHYLBUTYLBENZENE (sec AMYLBENZENE)	4.73	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1,2,3,5-TETRAMETHYLBENZENE 9.26 0.00%	3.4 DIMETHYI CUMENE	8.90	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	_
2)3/30 TERMETHYLENE 2130 01004 </td <td>1 2 3 5-TETRAMETHYLBENZENE</td> <td>9.26</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0.00%</td> <td>0 15%</td>	1 2 3 5-TETRAMETHYLBENZENE	9.26	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0 15%
1,2,3,4-TETRAMETHYLBENZENE 9.26 0.01% 0.00%	TERT-1-BLIT-2-METHYLBENZENE	4 73	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
12.9.7 11.0	1 2 3 4-TETRAMETHYI BENZENE	9.26	0.02%	0.00%	0.00%	0.00%	0.00%	0.01%	0.00%	0.09
TERT-1-BUT-3,5-DIMETHYLBENZENE 8.02 0.00%	N-PENT-BENZENE	2 12	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
TERT-1-BUTYL-4-ETHYLBENZENE 3.88 0.00% <td< td=""><td>TERT-1-BUT-3 5-DIMETHYI BENZENE</td><td>8.02</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.00%</td><td>0.02%</td><td>0.00%</td><td>-</td></td<>	TERT-1-BUT-3 5-DIMETHYI BENZENE	8.02	0.00%	0.00%	0.00%	0.00%	0.00%	0.02%	0.00%	-
NAPHTHALENE 3.34 0.00%	TERT-1-BUTYI -4-FTHYI BENZENE	3.88	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
DODECANE 0.55 0.02% 0.00% <	NAPHTHAIFNE	3 34	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.03%
1,3,5-TRIETHYLBENZENE 7.30 0.00%	DODECANE	0.55	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
1,2,4-TRIETHYLBENZENE 7.30 0.00%		7 30	0.02%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
HEXYLBENZENE 1.90 0.00%	1 2 4-TRIFTHYI BENZENE	7.30	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
Interfact in the interfact interfact in the interfact interfact in the interfact inte		1 90	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	
Formaldehyde 9.46 0.41% 0.17% 0.00% 0.45% 0.16% 0.52% 0.00% 0.87% Acetaldehyde 6.54 0.27% 0.08% 0.24% 1.26% 0.08% 1.48% 0.12% 1.61% Acrolein 7.45 0.08% 0.00% 0.00% 0.07% 0.00% 0.07% 0.00% 0.07% 0.00% 0.07% Acetone 0.36 0.24% 0.25% 0.48% 0.21% 0.81% 0.27% 0.06% 0.35% Propionaldehyde 7.08 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.05% Crotonaldehyde 9.39 0.02% 0.25% 0.08% 0.01% 0.44% - N-buttvraldebyde 5.97 0.02% 0.08% 0.01% 0.04% - 0.01%		0.86	3 36%	2.80%	2 39%	1 01%	1 20%	1 57%	0.00%	2 18%
Acetaldehyde 6.54 0.27% 0.08% 0.24% 1.26% 0.08% 1.48% 0.12% 1.61% Acetaldehyde 6.54 0.27% 0.08% 0.24% 1.26% 0.08% 1.48% 0.12% 1.61% Acrolein 7.45 0.08% 0.00% 0.00% 0.07% 0.00% 0.07% 0.00% 0.07% 0.00% 0.07% Acetone 0.36 0.24% 0.25% 0.48% 0.21% 0.81% 0.27% 0.06% 0.35% Propionaldehyde 7.08 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.05% Crotonaldehyde 9.39 0.02% 0.25% 0.08% 0.01% 0.44% - N-buttvraldebyde 5.97 0.02% 0.08% 0.01% 0.04% - 0.01%	Formaldebyde	9.00	0.41%	0.17%	0.00%	0.45%	0.16%	0.52%	0.44%	0.87%
Acrolein 7.45 0.08% 0.00% 0.07% 0.00% 0.12% 1.10% Acrolein 7.45 0.08% 0.00% 0.07% 0.00% 0.07% 0.00% 0.07% Acetone 0.36 0.24% 0.25% 0.48% 0.21% 0.81% 0.27% 0.06% 0.05% Propionaldehyde 7.08 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.05% Crotonaldehyde 9.39 0.02% 0.25% 0.08% 0.01% 0.44% - N-buttvraldebyde 5.97 0.02% 0.08% 0.01% 0.09% 0.01%	Acetaldebyde	6 5/	0.77%	0.17%	0.30%	1.26%	0.10%	1 /18%	0.00%	1 61%
Acetone 0.36 0.24% 0.25% 0.48% 0.21% 0.81% 0.27% 0.06% 0.03% Propionaldehyde 7.08 0.03% 0.00% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.05% Crotonaldehyde 9.39 0.02% 0.25% 0.00% 0.01% 0.04% - 0.01% 0.04% - 0.01%	Acrolein	7 /5	0.27%	0.00%	0.24%	0.07%	0.00%	0.07%	0.12/0	0.07%
Propionaldehyde 7.08 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.01% 0.04% 0.01% 0.00% 0.01% 0.01% 0.00% 0.01% 0.01% 0.00% 0.01%	Acetone	0.35	0.08%	0.00%	0.00%	0.07%	0.00%	0.07%	0.00%	0.07%
Crotonaldehyde 9.39 0.02% 0.25% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.00% 0.03% 0.01% 0.00% 0.01% 0.01% 0.00% 0.01%	Pronionaldehyde	7 00	0.24%	0.23%	0.40%	0.21%	0.01%	0.27/0	0.00%	0.33%
N-butyraldehyde 5.97 0.02% 0.00% 0.01% 0.01% 0.044% -	Crotonaldehyde	0.00	0.05%	0.00%	0.00%	0.03%	0.00%	0.05%	0.00%	0.05%
	N-hutvraldebyde	5.07	0.02%	0.23%	0.00%	0.01%	0.08%	0.01%	0.44%	- 0.01%

SENVIRON

May 2015 FINAL REPORT

		Fuel 1	Fuel 1	Fuel 1	Fuel 2	Fuel 2	Fuel 3	Fuel 3	EPA Profile
Compound	MIR	Bag 1	Bag 2	Bag 3	Bag 1	Bag 3	Bag 1	Bag 3	8757
Methyl Ethyl Ketone	1.48	0.05%	0.00%	0.48%	0.07%	0.40%	0.06%	0.00%	0.01%
Benzaldehyde	-0.67	0.16%	0.17%	0.00%	0.10%	0.00%	0.10%	0.00%	0.17%
Isovaleraldehyde	4.97	0.01%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-
Valeraldehyde	5.08	0.00%	0.00%	0.00%	0.03%	0.85%	0.00%	0.00%	0.04%
Tolualdehydes	0.00	0.01%	0.00%	0.00%	0.01%	0.00%	0.01%	0.00%	0.02%
Methylbenzaldehyde		0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.04%
Hexanaldehyde	4.35	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.04%
Dimethylbenzaldehyde	0.01	0.00%	0.00%	0.00%	0.00%	0.00%	0.01%	0.12%	0.00%
Methanol	0.67	0.29%	0.08%	1.44%	0.41%	1.69%	0.30%	1.24%	0.54%
Ethanol	1.53	0.01%	0.00%	0.00%	4.27%	0.00%	7.21%	0.31%	3.81%
2-Propanol	0.61	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.64%
1-Propanol	2.50	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	-

NOTE A - 2,2-Dimethylpentane and methylcyclopentane co-elute. Gas chromatography (GC) peak area split equally between the two compounds.

NOTE B - 3-Methyl-3-ethy-pentane co-elutes with reported compound. Not reported separately.

NOTE C - Cis-1,4-Dimethylcyclohexane co-elutes with reported compound. Not reported separately.

NOTE D - Propylcyclopentane co-elutes with reported compound. Not reported separately.

NOTE E - 2,5-Dimethylheptane and 3,5-dimethylheptane co-elute. GC peak area split equally between the two compounds.

NOTE F - Decane and isobutylbenzene co-elute. GC peak area split equally between the two compounds.

NOTE G - n-Butylbenzene co-elutes with reported compound. Not reported separately.

NOTE H - Isobutyraldehyde and methyl ethyl ketone co-elute. Liquid chromatography (LC) peak area split equally between the two compounds.



					Fuel 1			Fuel 2		Fuel 3			
Code	Make	Model	Test	Bag 1	Bag 2	Bag 3	Bag 1	Bag 2	Bag 3	Bag 1	Bag 2	Bag 3	
CCOB	Chevrolet	Cobalt	T1	94%	20%	11753%	111%	30%	132%	100%	44%	105%	
CCOB	Chevrolet	Cobalt	T2	6%	4%	1%	12%	0%	1%	18%	0%	0%	
CCOB	Chevrolet	Cobalt	T3										
CIMP	Chevrolet	Impala	T1	94%	63%	76%	106%	70%	50%	104%	70%	88%	
CIMP	Chevrolet	Impala	T2	9%	7%	12%	16%	3%	0%	21%	9%	8%	
CIMP	Chevrolet	Impala	T3										
CSIL	Chevrolet	Silverado	T1	8%	4%	7%	139%	140%	109%	123%	74%	101%	
CSIL	Chevrolet	Silverado	T2	108%	96%	78%	13%	6%	6%	23%	4%	30%	
CSIL	Chevrolet	Silverado	Т3							20%	3%	3%	
DCAL	Dodge	Caliber	T1	99%	67%	99%	111%	28%	88%	124%	40%	109%	
DCAL	Dodge	Caliber	T2	8%	12%	13%	15%	3%	11%	20%	4%	12%	
DCAL	Dodge	Caliber	Т3										
F150	Ford	F150	T1	8%	11%	6%	113%	151%	92%	109%	71%	64%	
F150	Ford	F150	T2	102%	138%	63%	15%	8%	16%	14%	7%	31%	
F150	Ford	F150	T3	10%	14%	8%							
FEXP	Ford	Explorer	T1	101%	52%	28%	114%	47%	77%	113%	71%	244%	
FEXP	Ford	Explorer	T2	7%	4%	12%	14%	2%	N/A	17%	0%	0%	
FEXP	Ford	Explorer	Т3							17%	0%	0%	
HODY	Honda	Odyssey	T1	106%	123%	N/A	114%	8%	133%	135%	12%	N/A	
HODY	Honda	Odyssey	T2	6%	0%	0%	12%	1%	N/A				
HODY	Honda	Odyssey	T4							17%	0%	0%	
NALT	Nissan	Altima	T1	97%	100%	58%	101%	51%	58%	106%	51%	N/A	
NALT	Nissan	Altima	T2	6%	23%	27%	12%	5%	109%	10%	7%	N/A	
NALT	Nissan	Altima	T3										
SOUT	Saturn	Outlook XE	T1	4%	2%	4%	122%	51%	46%	123%	31%	59%	
SOUT	Saturn	Outlook XE	T2	4%	3%	8%	15%	4%	0%	112%	31%	26%	
SOUT	Saturn	Outlook XE	T3	103%	48%	77%							
TCAM	Toyota	Camry	T1	99%	17%	143%	109%	32%	178%	112%	25%	N/A	
TCAM	Toyota	Camry	T2	5%	2%	78%				20%	3%	N/A	
TCAM	Toyota	Camry	Т3				13%	0%	5%				
TCOR	Toyota	Corolla	T1	93%	131%	171%				109%	1181%	73%	
TCOR	Toyota	Corolla	T2	5%	1%	N/A	105%	43%	120%	18%	0%	28%	
TCOR	Toyota	Corolla	Т3				13%	0%	N/A	20%	1%	N/A	
TSIE	Toyota	Sienna	T1	99%	24%	N/A				115%	29%	71%	
TSIE	Toyota	Sienna	T2	7%	1%	N/A	111%	13%	356%				
TSIE	Toyota	Sienna	Т3				15%	0%	0%	20%	0%	N/A	
FFOC	Ford	Focus	T1	89%	N/A	47%	100%	20%	74%	100%	37%	N/A	
FFOC	Ford	Focus	T2	14%	17%	5%	18%	N/A	0%	18%	3%	N/A	
FFOC	Ford	Focus	Т3										
HCIV	Honda	Civic	T1	93%	N/A	82%	100%	42%	N/A	116%	N/A	1034%	
HCIV	Honda	Civic	T2	8%	117%	13%	16%	3%	N/A	20%	N/A	4%	
HCIV	Honda	Civic	T3										
JLIB	Jeep	Liberty	T1	100%	75%	91%	110%	97%	118%	111%	104%	172%	
JLIB	Jeep	Liberty	T2	9%	0%	3%	14%	2%	2%	19%	6%	11%	
JLIB	Jeep	Liberty	T3										

Table A-2. Speciation recovery fraction (Sum of speciation/NMHC) of test results.