Motor Vehicle Emission Factor Model

MOBILE6.2 Air Toxic

Trend and Sensitivity Analysis

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ABSTRACT

The newly released MOBILE6.2 has incorporated both air toxic and particulate matter emission factor modeling functions. A series of test runs were performed to gain a better understanding of the air toxic modeling function and overall model behavior. These test runs/scenarios evaluated the changes in emission factors of all six built in air toxic compounds as affected by vehicle activities, fuel physical properties, fuel chemical compositions, oxygenated fuel additives, and environmental conditions. Based on results obtained, both exhaust and evaporative emission factors for acrolein, acetaldehyde, benzene, 1,3 butadiene, formaldehyde, methyl tertiary butyl ether are inversely proportional to both freeway and arterial vehicle speeds. This phenomenon follows the trend of total organic gas emission factors. Effects from roadway facility differences indicated that the higher the percentage of vehicle miles traveled on a freeway, the lower the air toxic emission factors on a per vehicle mile traveled basis. Both exhaust and evaporative air toxic emission factors increase when fuel RVP value and sulfur content increase. It is interesting to note that diesel sulfur content has no effect on the six toxic compound emission factors. Effects from fuel chemical compositions on all emission factors varied. However, chemical compositions do have significant effects on all air toxic compound emission factors. On the same note, both min/max temperatures and humidity affect all air toxic emissions significantly. The time series evaluation shows that all six tested air toxic compound emissions decrease linearly from year 2002 to 2020.

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INTRODUCTION

Since the official release of the MOBILE6.0-motor vehicle emission factor modeling program by the US EPA on January 29, 2002, two updated versions known as MOBILE6.2.01 and MOBILE6.2.03 have been released. MOBILE6.2 has functions of estimating both air toxic and particulate emission factors in addition to all functions contained in MOBILE6.0. According to EPA's technical guidance, MOBILE6.2's air toxic function is a consolidation of an earlier hazardous air pollutant estimation model known as MOBTOX to MOBILE6.0. With the robust capability of the MOBILE6 model, it appears that this new function can evaluate effects of more specific vehicle activities, environmental conditions, fuel properties, and other parameters on air toxic emissions. The objective of this analysis is to explore the effects of various parameters and conditions on emission factors of compounds built into the air toxic module of the MOBILE6.2 model. These six built-in air toxic compounds are acrolein, acetaldehyde, benzene, 1,3 butadiene, formaldehyde, and methyl tertiary butyl ether (MTBE). Evaluation of diesel particulate matter (DPM) emission behavior as affected by various vehicle and environmental conditions through MOBILE6.2 is reported separately from this study.

METHODOLOGY

For all modeling runs, optional data (not associated with required MOBILE6 Commands) other than those being tested were based on MOBILE6 national defaults. For all scenarios, the modeling year (calendar year) was 2005. Fuel Reid Vapor Pressure (RVP) used for all runs except in RVP testing was 8.5 pounds per square inch (psi). Min/Max temperatures were 88.0 degrees Fahrenheit and 100.0 degrees

Fahrenheit except in the case of min/max temperature testing. Other conditions as listed below were also applied to all scenarios when appropriate. Volume based gas aromatic, olefin, and benzene contents (v/v) were 15.0% (v/v), 15.0% (v/v), and 1.5% (v/v), respectively; E200 was 50.0% (v/v) while E300 was100.0% (v/v). Oxygenated fuel consisted of 8.0% (v/v) MTBE with a 1.0% market share, 10% (v/v) ethyl tertiary butyl ether (ETBE) with a 1.0% market share, 5.0% ethanol (ETOH) (v/v) with a 1.0% market share, and 1.0% tertiary amyl methyl ether (TAME) (v/v) with a 1.0% market share.

Emission factor data for all the six air toxic compounds were plotted on a single graph for a given tested parameter in order to conduct trend analysis. Raw data for one or more emission factors on the graph were scaled either up or down. For example, benzene data in a given graph were scaled up by multiplying all data points by three. In this case, the legend for benzene in the graph would be benzene*3. The true emission factor for benzene in this graph is equal to the graph value divided by three. By conducting the above scale up or down operations, trend deviation and pattern development are more decipherable. Units for all air toxic compounds are milligram per vehicle miles traveled (mg/mi). The unit for Total Organic Gas (TOG) emission factor is gram per mile (g/mi).

Tested parameters are categorized into the following groups: 1) vehicle activities such as vehicle speed and VMT ratio, 2) fuel physical properties such as Reid Vapor Pressure (RVP), 3) fuel chemical compositions such as benzene content, aromatic content, olefin content, sulfur content, E200, and E300 contents, 4) other chemical additives used in oxygenated fuel, 5) environmental factors such as min/max temperatures, and 6) time series data for calendar years between 2002 and 2020.

RESULTS AND DISCUSSION

Vehicle Speed

The "AVERAGE SPEED" command was used to evaluate both arterial and freeway mainline speed effects. Speeds ranging from 2.5 to 65.0 miles per hour (mph) with a 2.5 mph increment were tested.

Fig. 1 shows the relationship between exhaust emission factors and freeway mainline speeds. It is clear from Fig.1 that emission factors for all six air toxic compounds are following the trend of TOG emission. Between 2.5 and 22.5 mph, the relationship can be approximated by an exponential function. Emission factors decrease rapidly as vehicle speeds approach 22.5 mph. Between 22.5 and 65.0 mph, all exhaust air toxic emission factors decrease in a flat linear fashion. The higher the speed, the lower the exhaust emission factor.

Figure 1 Freeway Facility Speed Effects on Exhaust Toxic Emissions

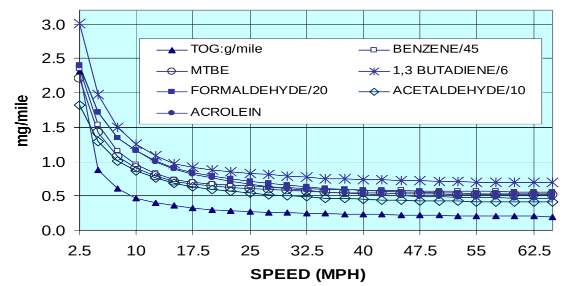
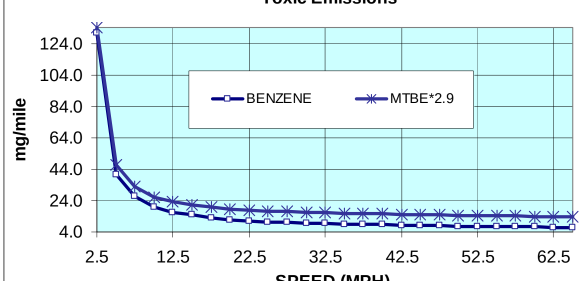


Fig. 2 depicts the relationship between evaporative air toxic compound emission factors and freeway mainline speeds. Unlike the exhaust emission trend, the initial rapid decrease of evaporative emission stops at 5.0 mph. The second rapid decrease occurs between 5.0 and 12.5 mph. Between 12.5 and 65.0 mph, the relationship between evaporative emission and vehicle speed can be described through a linear model. Again, the higher the speed becomes, the lower the emission factor.

Figure 2 Freeway Facility Speed Effects on Evaporative Toxic Emissions



The relationship between exhaust emission factor and arterial roadway is essentially a duplicate of the emission factor/freeway facility correlation (Figs. 3 & 4). It clearly shows that roadway facility speed is the major factor leading to exhaust air toxic emission factor differences.

Figure 3 Arterial Facility Speed Effects on Exhaust Toxic Emissions

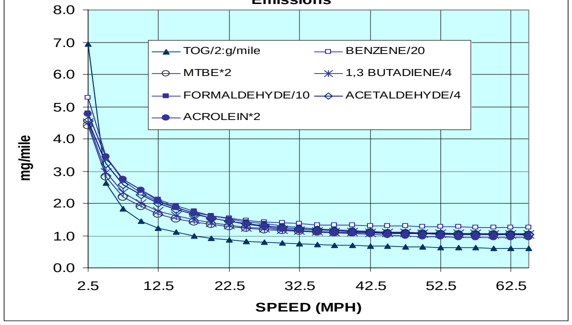
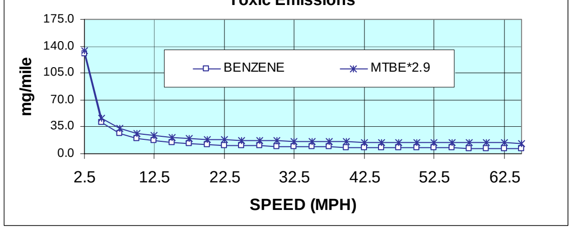


Figure 4 Arterial Facility Speed Effects on Evaporative Toxic Emissions



VMT Ratio

Effects of vehicle miles traveled (VMT) ratios between different roadway facilities were evaluated by using the command of “VMT BY FACILITY” and appropriate external VMT files. Tested VMT ratios between freeway mainline/arterial and arterial/local were from 0.0% to 100.0%. The objective of this test is to understand how critical it is to accurately allocate VMT among all roadway types during transportation demand modeling and forecasting.

Fig.5 depicts effects of VMT ratio between an arterial roadway and a local facility on emission factors of all exhaust air toxic compounds and TOG. Clearly, relationships between VMT ratios and emission factors are linear for all exhaust emissions. The higher the percentage of the VMT on a local road, the higher the exhaust air toxic emission factor. Effects of VMT ratio between a freeway mainline and an arterial facility on air toxic emissions are similar in trend but less pronounced in magnitude as compared with the arterial/local VMT ratio effects (Fig. 7). Vehicles traveling a freeway produce lower air toxic emission factors than vehicles traveling an arterial facility on a per mile traveled basis.

Evaporative benzene and MTBE emission factors are also linearly related to VMT ratios (Fig. 6 & 8) for both cases.

Figure 5 VMT Ratio (ARTERIAL/LOCAL) Effects on Exhaust Toxic Emissions

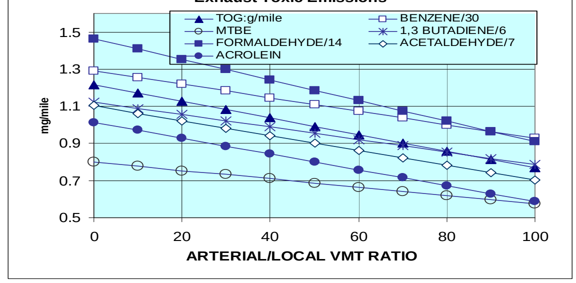


Figure 6 VMT Ratio (ARTERIAL/LOCAL) Effects on Evaporative Toxic Emissions

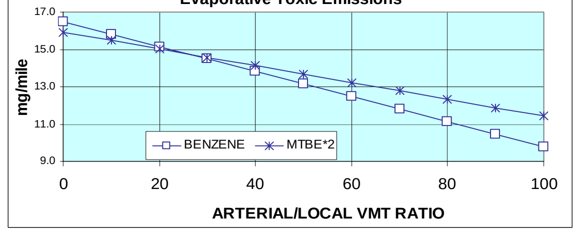


Figure 7 VMT Ratio (Freeway/Arterial) Effect on Exhaust Toxic Emissions

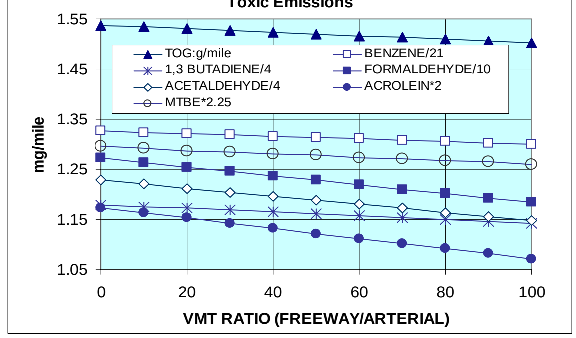
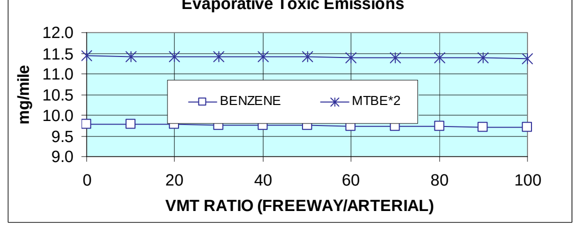


Figure 8 VMT Ratio (Freeway/Arterial) Effects on Evaporative Toxic Emissions



Fuel Reid Vapor Pressure

Fuel Reid Vapor Pressure (RVP) is one of the few required inputs to run MOBILE6. While it is known that a high RVP fuel produces high amounts of evaporative and exhaust VOC emissions, it is not clear how RVP affects air toxic emissions. The objective for the RVP test is to understand how air toxic emissions are influenced by fuel RVP changes. Effects from fuel RVP ranging from 6.5 to 15.5 psi were evaluated.

Fig. 9 outlines the RVP effects on all six air toxic compounds and TOG exhaust emissions. As fuel RVP increases, TOG emission factors increase with different rates depending on the range of RVP data. Unlike the TOG emission trend, the air toxic compound exhaust emissions exhibit three distinctively different trends. Between 6.5 and 8.5 psi, air toxic compound emission factors decease in a linear fashion as fuel RVP increases. Between 8.5 and 12.5 psi, the air toxic compound emission factors increase with increasing fuel RVP value. Once the fuel RVP value exceeds 12.5 psi, benzene, formaldehyde, and 1,3 butadiene emission factors start to decrease again as fuel RVP increases. The acetaldehyde, acrolein, and MTBE emission factors remain unaffected while the TOG emission factor increases at a lower factor.

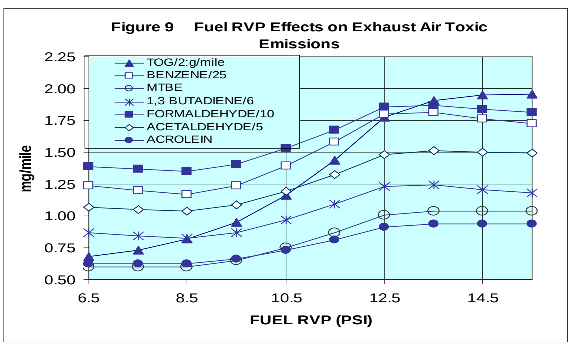


Figure 9 Fuel RVP Effects on Exhaust Air Toxic Emissions

Fig.10 shows the evaporative benzene and MTBE emission trends. As fuel RVP increases, both benzene and MTBE emission factors increase although MTBE does not increase as rapidly as benzene

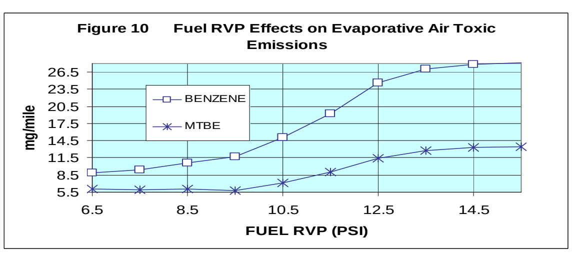


Figure 10 Fuel RVP Effects on Evaporative Air Toxic Emissions

Gasoline Sulfur Effects

The MOBILE6 command "FUEL PROGRAM" was used to evaluate effects of gasoline sulfur (ranging from 32 to 92 ppm) on exhaust air toxic emission factors.

Based on results showed in Fig. 11, all exhaust toxic air compound emission factors increase linearly as gasoline sulfur increases. It appears that all air toxic compound emissions follow the TOG emission trend.

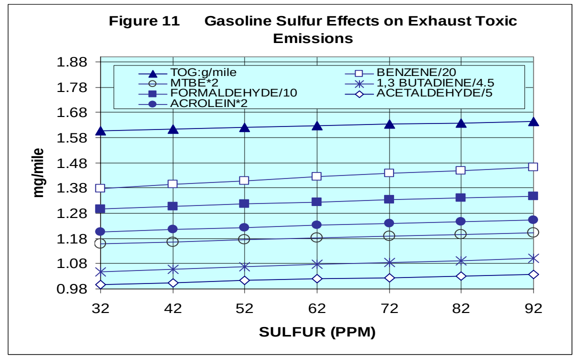


Figure 11 Gasoline Sulfur Effects on Exhaust Toxic Emissions

Gasoline sulfur content has no effect on evaporative air toxic compound emissions.

Diesel Sulfur Effects

Diesel sulfur content has no effect on emissions of all six air toxic compound emissions tested here.

E200 Effects

E200 is a gasoline volatility measurement. It is the volume percentage of a given amount of gasoline that evaporates at 200 degrees Fahrenheit under one atmospheric pressure. The range of E200 tested was between 30.0% and 70.0%

According to Fig. 12, exhaust TOG, MTBE and acrolein emissions are not affected by E200 contents. Exhaust benzene emissions increase slightly when E200 increases from 35.0% to 45.0%. Between 45.0% and 70.0% E200 contents, exhaust benzene emissions decrease rapidly as E200 content increases. Emission factors for both formaldehyde and

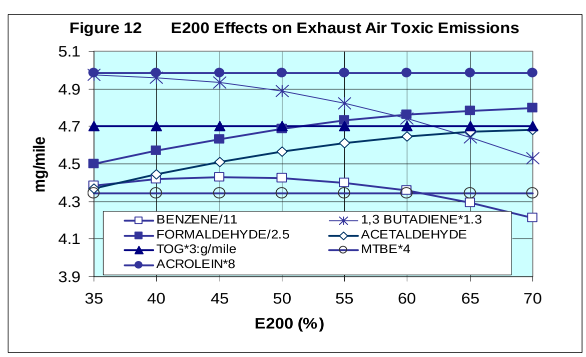


Figure 12 E200 Effects on Exhaust Air Toxic Emissions

acetaldehyde increase as the E200 content increases.

One of the most dramatic phenomena is the decreasing of 1, 3-butadiene emission as the content of E200 increases. As E200 content increases (the content of lower molecular weight distillates increase), more of the relatively large 1,3 butadiene is produced.

E200 content has no effects on evaporative benzene and MTBE emissions.

E300 Effects

E300 is another measurement of gasoline volatility. It is the volume percentage of a given amount of gasoline evaporated at 300 degrees Fahrenheit under one atmospheric pressure. The range of E300 tested was from 70.0% to 100.0%.

Exhaust benzene emission (Fig. 13) increases rapidly with increasing E300 content. This observation is just the opposite of the E200 result.

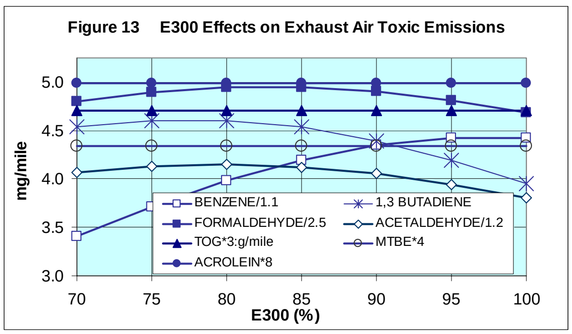


Figure 13 E300 Effects on Exhaust Air Toxic Emissions

Formaldehyde, acetaldehyde and 1,3 butadiene exhaust emissions increase as E300 increases from 70.0% to 80.0%. Between 80.0% and 100.0%, the emission factors for these three compounds decrease as E300 increases.

Acrolein, MTBE and TOG emission factors are not affected by E300 contents. This observation is consistent with the E200 data.

Evaporative emission factors for both MTBE and benzene are not affected by E300 changes. This result is the same as the E200 results.

Aromatic Effects

Aromatic compounds are any compounds that possess the six-carbon ring (benzene) structure. Effects of aromatic content on air toxic compound production were evaluated by using the command of “Gas Aromatic%.” Aromatic contents ranging from 10.0% to 55.0% were evaluated while benzene content was fixed at 1.5%.

Exhaust emission factors for TOG, acrolein, and MTBE are not affected by the contents of aromatic compounds (Fig. 14). However, exhaust benzene emission factor increase rapidly in a virtually linear mode as the aromatic content increases.

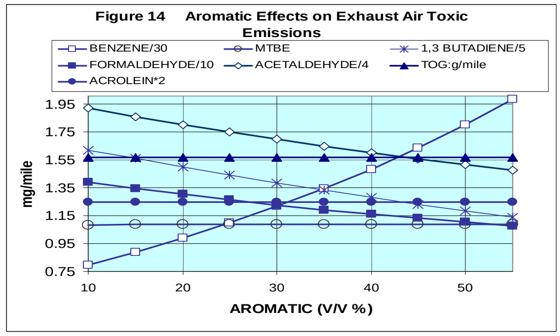


Figure 14 Aromatic Effects on Exhaust Air Toxic Emissions

While exhaust benzene emission factors increase with increasing aromatic contents, butadiene, formaldehyde, and acetaldehyde emissions decrease in a linear fashion.

Evaporative emission factors for both benzene and MTBE are not affected by the amounts of aromatic compounds in fuel.

Benzene Effects

While benzene is one of many compounds referred to as aromatic, it is the only reported air toxic chemical among all aromatic compounds. Effects of benzene ranging from 0.0% to 5.0% were analyzed.

As benzene content increases from 0.0% to 5.0%, exhaust benzene emissions increase

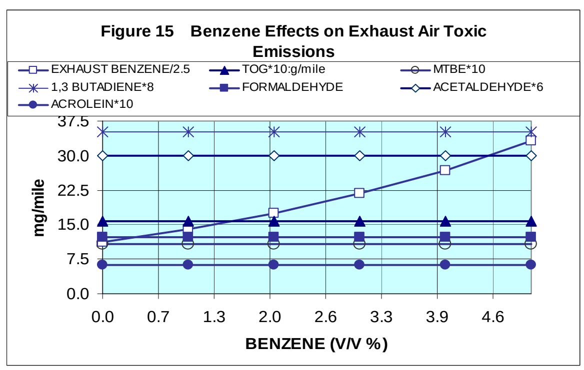


Figure 15 Benzene Effects on Exhaust Air Toxic Emissions

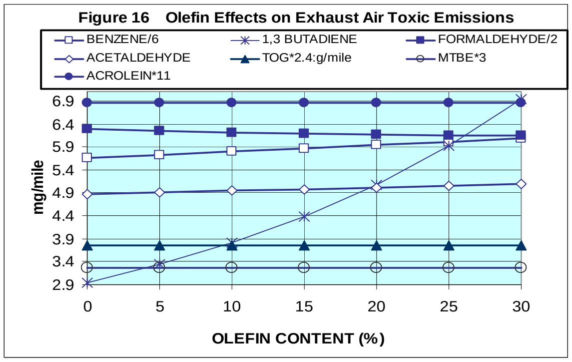
linearly (Fig. 15). This same linear response is also observed with the evaporative benzene emission factors. No other air toxic compound emission factors are affected by benzene content.

Olefin Effects

Olefin refers to a class of compounds containing either double or triple bonds. Effects of olefin content ranging from 0.0% to 30.0% on the production of air toxic compounds were analyzed.

Exhaust air toxic emissions as affected by olefin contents are shown in Fig. 16. While 1,3 butadiene emission factor increases rapidly with increasing olefin content, acetaldehyde and benzene emission factors increases are less obvious. On the other hand, formaldehyde emission factor decreases as olefin content increases.

Figure 16 Olefin Effects on Exhaust Air Toxic Emissions



MTBE and benzene evaporative emissions are not affected by olefin content.

Oxygenated Fuel Effects

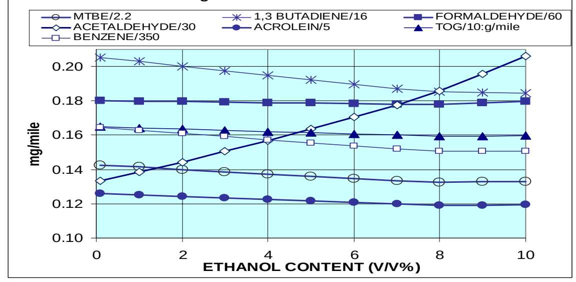
To evaluate effects from fuel additives used in oxygenated fuel blending, the MOBILE6 command “OXYGENATE” was used. For each additive, a 70.0% market share was used.

Ethanol

The ethanol contents ranging from 0.0% to 10.0% volume (v/v) were analyzed for their effects on air toxic emissions.

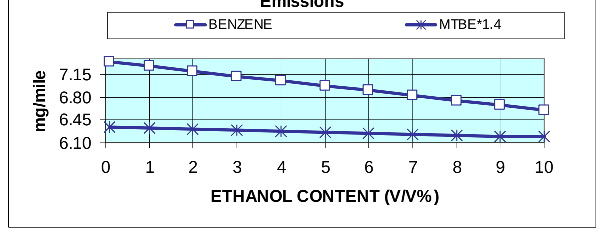
Exhaust emission factors for all air toxic compounds except acetaldehyde decrease as ethanol content increases (Fig. 17). This decreasing trend is also true with TOG emissions. This phenomenon may be contributed to the direct oxidation of ethanol to acetaldehyde during the combustion process.

Figure 17 ETHANOL Effects



According to Fig. 18, as more ethanol is blended in the fuel, evaporative emissions of both benzene and MTBE decrease. This phenomenon is especially true for evaporative benzene emissions.

Figure 18 ETHANOL Effects on Evaporative Air Toxic Emissions



MTBE

The blending volume percentages for MTBE ranging from 0.0% to 14.5% were used in analyzing MTBE effects on air toxic emission (Figs. 19&19a). Exhaust emission factors for all toxic compounds except formaldehyde decrease linearly as MTBE content increases.

Figure 19 MTBE Effects on Exhaust Air Toxic Emissions

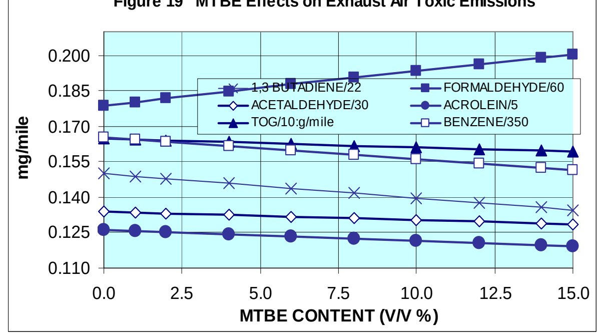
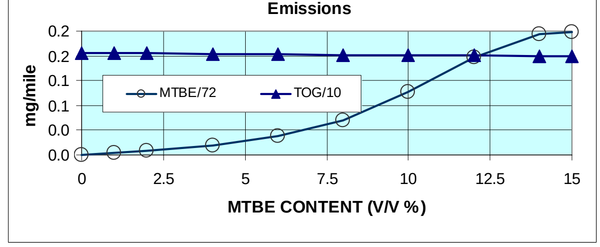


Figure 19a MTBE Effects on Exhaust Air Toxic Emissions



Evaporative benzene emission factors decrease as MTBE content increases (Fig. 20).

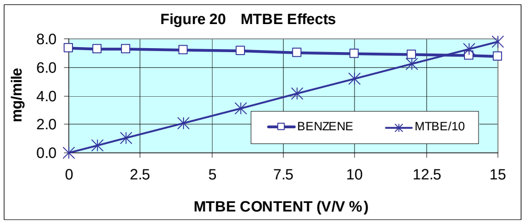


Figure 20 MTBE Effects

ETBE

The blending volume percentages for ETBE ranging from 0.0% to 16.0% were used to evaluate ETBE effects on air toxic emission. Similar patterns as ethanol affecting air toxic emissions are observed (Fig. 21). As ETBE content increases, all air toxic emissions except acetaldehyde decrease. This is a very interesting discovery since ETBE belongs to ether family and not the alcohol.

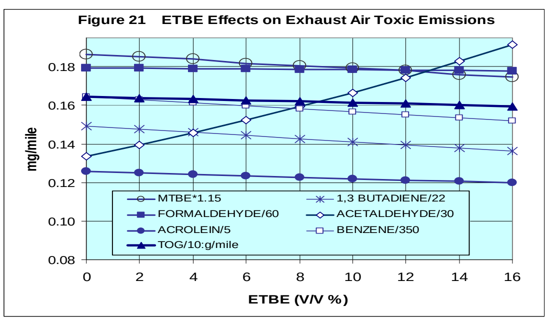


Figure 21 ETBE Effects on Exhaust Air Toxic Emissions

For both evaporative and exhaust emissions, similar patterns as EOTH affecting air toxic emissions are observed (Figs. 22).

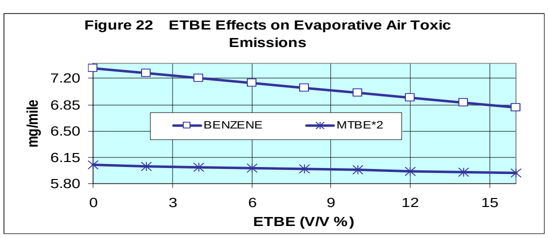


Figure 22 ETBE Effects on Evaporative Air Toxic Emissions

TAME

The blending volume percentages for TAME ranging from 0.0% to 18.0% were analyzed for their impacts on air toxic emissions. While effects from ETBE resemble the ethanol effect, effects from TAME on all air toxic emissions resemble the MTBE impact. Formaldehyde emission factors increase in a linear fashion as TAME content increases while all other air toxic emission factors decrease (Figs. 23 & 24).

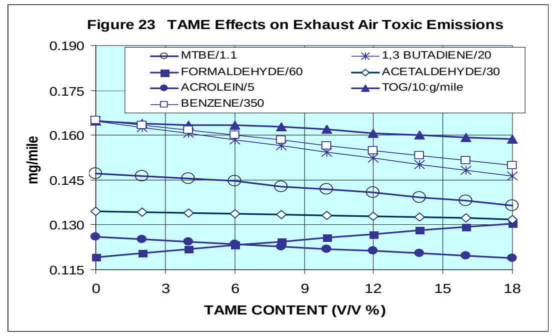


Figure 23 TAME Effects on Exhaust Air Toxic Emissions

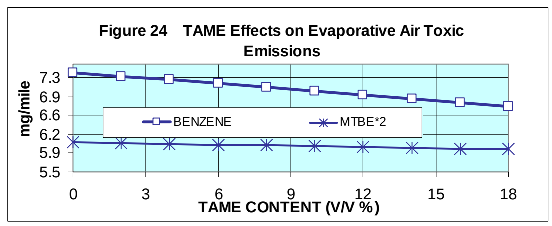


Figure 24 TAME Effects on Evaporative Air Toxic Emissions

Environmental Factors

Effects from environmental factors including minimum/maximum daily temperatures and humidity were evaluated for their impacts on air toxic emissions. While testing minimum temperature effects, maximum daily temperature was held at 70 degrees Fahrenheit. The minimum daily temperature was held at 80 degrees Fahrenheit, while daily maximum temperature effects were evaluated.

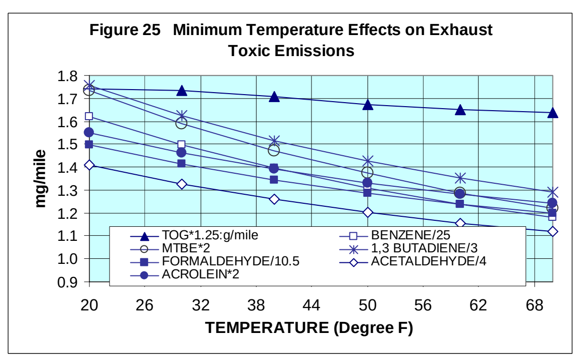


Figure 25 Minimum Temperature Effects on Exhaust Toxic Emissions

As indicated in Fig. 25, all exhaust air toxic compounds and TOG emissions increase as daily minimum temperature decreases. All emission factors are virtually parallel to each other. As the daily maximum temperature increases, all exhaust emissions increase (Fig. 26). However, all air toxic compound emissions are at a much lower rate than the TOG emission factor.

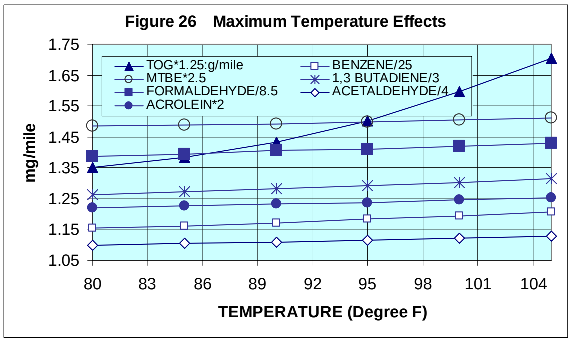


Figure 26 Maximum Temperature Effects

On other hand, evaporative emissions of both benzene and MTBE decrease as daily minimum temperature decreases (Fig 27). Evaporative emissions of both benzene and MTBE increase as daily maximum temperature increases (Fig.28).

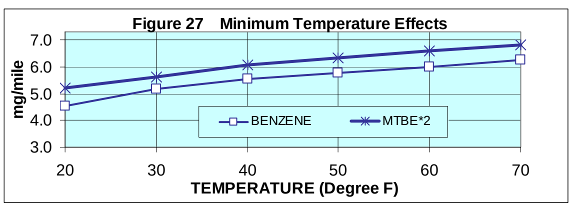


Figure 27 Minimum Temperature Effects

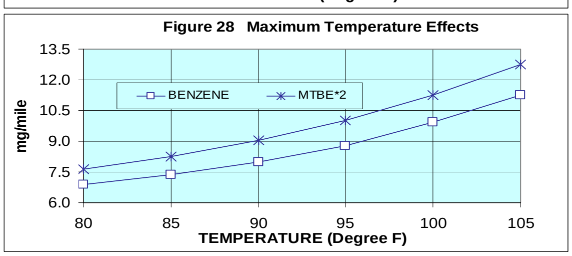


Figure 28 Maximum Temperature Effects

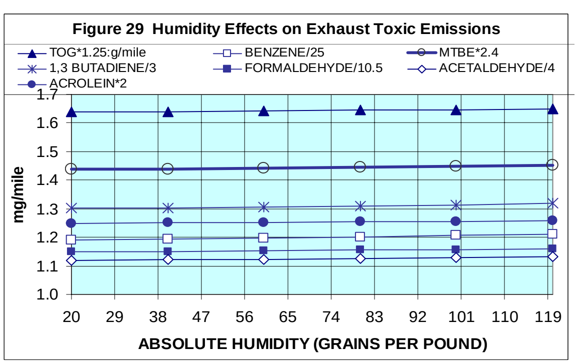


Figure 29 Humidity Effects on Exhaust Toxic Emissions

Humidity impacts on air toxic emissions are shown in Fig. 29. As humidity increases, all exhaust emissions including all air toxic compounds, MTBE and TOG increase at a similar factor. Humidity has no effect on evaporative emissions.

Time Series Analysis

By using default MOBILE6 data, a trend evaluation was carried out for calendar years between 2002 and 2020.

According to Fig. 30, exhaust emissions for all air toxic compounds and TOG are declining as time moves forward. This declining trend is essentially parallel to the TOG trend.

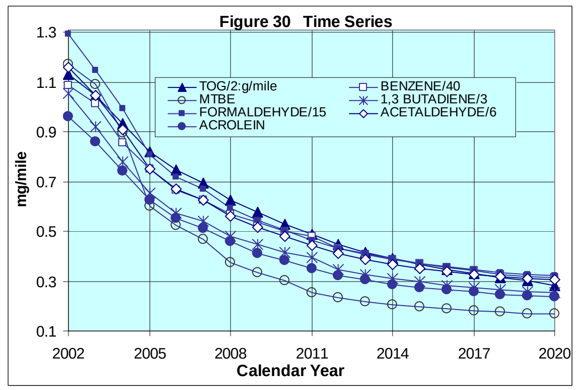


Figure 30 Time Series

Evaporative emission trends for both benzene and MTBE are also declining as time moves forward (Fig. 31). However, evaporative benzene emission factors decline at a much faster rate than MTBE.

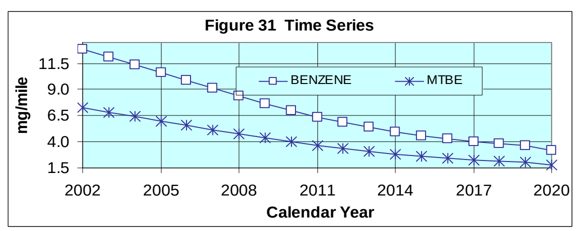


Figure 31 Time Series

SUMMARY

Effects of various parameters including vehicle, roadway facility, environment, and time on six different air toxic compound emissions and TOG were evaluated. While some parameters affected certain air toxic compounds significantly, others appeared to have no impacts. All impacts are grouped into six different categories, which are listed in the summary table below.

TABLE 1 Sensitivity Classification Summary

Tested Parameter	Exhaust*							Evaporative*	
	Acetaldehyde	Acrolein	Benzene	Butadiene	Formaldehyde	MTBE	TOG	Benzene	MTBE
Aromatic Content	♦♦	♦	♦♦♦	♦♦	♦♦	♦	♦	♦	♦
Arterial Speed (2.5-10.0 mph)	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦
Arterial Speed (10.0-22.5 mph)	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦
Arterial Speed (22.5-65.0 mph)	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦
Benzene Content	♦	♦	♦♦♦♦♦♦	♦	♦	♦	♦	♦♦♦♦♦♦	♦
E200 Content	♦♦	♦	♦	♦♦	♦	♦	♦	♦	♦
E300 Content	♦♦	♦	♦♦	♦♦	♦	♦	♦	♦	♦
ETBE Content	♦♦♦	♦♦	♦♦	♦♦	♦	♦♦	♦	♦♦	♦
Ethanol Content	♦♦♦	♦♦	♦♦	♦♦♦	♦	♦♦	♦♦	♦♦	♦♦
Freeway Speed (2.5-10.0 mph)	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦
Freeway Speed (10.0-22.5 mph)	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦	♦♦♦
Freeway Speed (22.5-65.0 mph)	♦♦	♦♦♦	♦♦	♦♦	♦♦	♦♦	♦♦♦	♦♦♦	♦♦
Gasoline Sulfur Content	♦	♦	♦	♦	♦	♦	♦	♦	♦
Humidity	♦	♦	♦	♦	♦	♦	♦	♦	♦
Maximum Temperature	♦	♦	♦	♦	♦	♦	♦♦♦	♦♦♦	♦♦♦
Minimum Temperature	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦	♦♦	♦♦
MTBE Content	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦♦♦♦	♦♦	♦♦	♦♦♦♦♦
Olefin Content	♦	♦	♦♦	♦♦♦♦	♦♦	♦	♦	♦	♦
RVP (6.5-8.5 PSI)	♦♦♦	♦	♦♦♦	♦♦♦	♦♦♦	♦♦	♦♦♦♦♦♦	♦♦♦♦♦	♦♦
RVP (8.5-12.5 PSI)	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦
RVP (12.5-15.0 PSI)	♦♦	♦♦	♦♦♦♦♦♦	♦♦♦♦♦♦	♦♦	♦♦♦	♦♦♦	♦♦♦♦	♦♦♦♦♦
TAME Content	♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦
VMT Ratio (Arterial/Local)	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦	♦♦
VMT Ratio (Freeway/Arterial)	♦	♦	♦	♦	♦	♦	♦	♦	♦

*Percentage change of an emission factor as a result of one unit increase of the tested parameter: ♦<0.2%; 0.2%<♦♦≤1.0%; 1.0%<♦♦♦ ≤4.0%; 4.0% <♦♦♦♦ ≤6.0%; 6.0% <♦♦♦♦♦ ≤10.0%; ♦♦♦♦♦♦>10.0%.

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NOTICE

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