DRAFT Final Report

The Case for a Dual Tech 4 Model Within the California Predictive Model

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For: Renewable Fuels Association (RFA)

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1. Executive Summary

On April 27, 2007, ARB released the Staff Report on Predictive Model revisions. The Staff report describes proposed revisions to the Predictive Model for certifying gasoline in California. The new procedures would take place starting on December 31, 2009.

The new Predictive Model incorporates a number of modifications from the previous model. The new model:

- Adds permeation VOC emissions to the model and requires the gasoline marketers to offset these increased emissions through gasoline recipe changes,
- Updates the motor vehicle emission inventory mix from 2005 to 2015
- Updates the reactivity adjustment factors,
- Adds new motor vehicle exhaust data, and
- Updates the effects of CO on ozone forming potential

In the process of updating the model, Staff considered suggestions by some stakeholders to divide the Tech 4 dataset (1986-1995 vehicles) into lower and higher emitter groups, and develop separate coefficients for these two groups. This is what we refer to as a "Dual Tech 4 model." Several analyses were presented showing improved correlations with the data when the data are separated by lower and higher emitters.

After considering a dual model for Tech 4 vehicles, staff concluded that it was not appropriate to use a dual model for Tech 4 vehicles. Reasons provided for this decision were:

- There are no physical response differences between vehicles emitting just below 0.6 times the NOx standard and those emitting just above 0.6 times the NOx standard,
- The alternative statistical method did not produce consistent results at the other pollutant cutpoints, and
- It is essential that emissions modeling be consistent with sound engineering judgment and good science and have a sound basis relative to vehicle control system design and combustion chemistry

However, the authors of this paper believe that staff and the stakeholders became overly focused on NOx and ethanol at the expense of the bigger picture with all fuel properties, and that there many reasons why a dual model for Tech 4 vehicles is a better model than a single model, and will result in better gasoline formulations in California when the new Predictive Model takes effect. First, addressing the above 3 issues, there are physical reasons why higher emitting vehicles have a different response than lower emitting vehicles. A lot of this has to do with catalyst efficiency – higher emitting vehicles have lower catalyst efficiency, so fuel properties that affect catalyst efficiency like sulfur and

ethanol should actually be *expected* to have a different response for lower emitters than for higher emitters. In addition to catalyst efficiency differences, normal emitters have relatively high cold start emissions and low warmed-up emissions, where higher emitters have higher emissions in all modes. Therefore, fuel properties that affect cold start emissions like distillation properties should be expected to have different percentage effects on higher than normal emitters.

The 0.6 factor was statistically determined from the data as the optimum cutoff for NOx, but even a cutoff of 1.0 times the standard was far superior to a single model. Second, we would have been extremely surprised if the alternative statistical method did produce consistent results at the other pollutant cutpoints. Thirdly, we agree that emission modeling be consistent with sound engineering judgment and good science, and believe that the dual model fulfills these requirements much better than the single model.

We believe that the staff and stakeholders have overlooked a very important fact about Tech 4 vehicles, and that is in 2015, the year of the new Predictive Model, most of the emissions will be from the higher emitting vehicles, and not from the lower emitting vehicles, in spite of the best efforts of the California I/M program. For example, the EMFAC model indicates that 70% of the NOx and 85% of the total organic gases (TOG) are from higher emitters. The single model was based on tests of Tech 4 vehicles performed over 10 years ago when these vehicles were very young. It is not appropriate to apply fuel relationships developed on very young vehicles to a very old Tech 4 vehicle population in 2015.

In this analysis, the authors developed a dual model for Tech 4 vehicles, and modified the Predictive Model accordingly. We also developed all the necessary weighting factors for lower and higher emitting Tech 4 vehicles, utilizing the latest EMFAC emissions model, EMFAC2007.

Results of a comparison of the dual and single models for Tech 4 vehicles show that when the dual model is used:

- NOx emissions increase less, and THC emissions decrease more when the oxygen weight fraction is increased from 2% to 3.5%. The reason for this is that catalyst efficiency on Tech 4 vehicles is low, so that a lean shift in the air fuel ratio of gases approaching the catalyst due to ethanol reduces THC emissions more, and has less effect on increasing NOx
- The effect of lowering T50 and T90 on reducing THC emissions is less because distillation properties primarily affect cold start emissions, and cold start emissions are a lower fraction of total emissions for higher emitters than for lower emitters
- The effect of lowering aromatics on THC emissions is increased because aromatics, with their high carbon to hydrogen ratio, richen the air:fuel ratio entering the catalyst, thus, lowering aromatics has a larger effect on higher emitting vehicles that have higher warmed-up emissions and less effective catalytic converters

All other fuel relationships are essentially the same as the ARB single model.

The staff report presents the model results of four example fuel that vary primarily in ethanol content. All four fuels in the staff report passed the new Predicitve Model. The results are shown in the table below.

When the dual model is used instead of the single model, the 0% ethanol fuel fails the dual model, the performance of the 5.7% ethanol fuel is about the same, and there is a a greater margin of performance with respect to OFP performance for the 7.7% and 10.0% ethanol fuels. For example, at 10% ethanol, the margin of performance for the dual model is -0.71%, while for the single model it is only -0.05%. The primary reasons for this is that the dual model reflects a greater reduction of HC emissions, and a lower increase in NOx emissions due to increasing ethanol content.

Table ES-1. Comparison of Single and Dual Model on Four Fuels Passing the ARB Single Model

	Percent Ethanol			
Property	0.0%	5.7%	7.7%	10.0%
RVP	6.60	6.91	6.92	6.99
T50	204	206	209	212
T90	315	310	313	313
Aromatic	25.0	25.0	25.0	25.0
Olefin	8.0	9.0	9.0	6.0
Total Oxygen	0.0	2.0	2.7	3.5
Sulfur	5	5	5	5
Benzene	0.50	0.50	0.50	0.50
Single Predictive Model Criteria	% Change in Emissions			
OFP	-0.67	-0.38	-0.59	-0.05
NOx	-6.0	-4.8	-2.9	-1.1
Pass/Fail	Pass	Pass	Pass	Pass
Dual Predictive Model Criteria	% Change in Emissions			
OFP	0.46	-0.25	-0.84	-0.71
NOx	-5.6	-4.8	-3.1	-1.5
Pass/Fail	Fail	Pass	Pass	Pass

The authors believe that the ARB should finalize the Predictive Model with the dual model for Tech 4, instead of the single model. Such a modification will be more technically correct, and would simultaneously provide greater flexibility for the oil industry to meet the Predictive Model requirements. Another good reason for using the dual model rather than the single model is that ARB uses the Predictive Model to develop fuel correction factors for fuels in EMFAC. The use of the dual model (or dual model

methodology) to develop these fuel correction factors will result in more accurate VOC, CO, and NOx inventories in California.

2. Introduction

On April 27, 2007, ARB released the Staff Report on Predictive Model revisions. [1] The Staff report describes proposed revisions to the Predictive Model for certifying gasoline in California. The new procedures would take place starting on December 31, 2009.

The new Predictive Model incorporates a number of modifications from the previous model. The new model:

- Adds permeation VOC emissions to the model and requires the gasoline marketers to offset these increased emissions through gasoline recipe changes,
- Updates the motor vehicle emission inventory mix from 2005 to 2015
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In the process of updating the model, Staff considered suggestions by some stakeholders to divide the Tech 4 dataset (1986-1995 vehicles) into lower and higher emitter groups, and develop separate coefficients for these two groups. This is what we refer to as a "Dual Tech 4 model." Several analyses were presented showing improved correlations with the data when the data are separated by lower and higher emitters.

ARB Staff considered this alternative. The following paragraphs repeat the Staff's discussion of this alternative:

> "During the workshop process, several stakeholders requested that the staff consider dividing the Tech 4 dataset into a higher and lower emitter group to be modeled separately, and presented the results of an analysis of dividing the datasets. The basic concept was that a Tech 4 NOx model would provide an overall higher statistical fit if the dataset were divided into two distinct vehicle groups. The cut point would be at 0.6 times the NOx emissions standard and each portion modeled separately. Proponents believe that this approach produces a much lower response of NOx to oxygen content and it would require less adjustment to other fuel properties to be able to increase the amount of ethanol into CARFG.
>
> Staff discussed this issue with the ARB's vehicle experts and consulted representatives of the Alliance of Automobile Manufacturers and the Association of International Automobile Manufacturers. These discussions focused on determining if there was some physical design factor in vehicle emission control systems that change how they respond to fuel property changes at the levels indicated by the stakeholder analysis. Staff learned that while many manufacturers do calibrate their emission control systems to emit at levels below the actual standard, there is no physical response differences between vehicles emitting just below 0.6 times the standard and those emitting just above 0.6 times the standard. This was important because the alternative statistical method did

not produce consistent results at other cut points. Lacking a technical reason for using the suggested 0.6, staff was concerned that the result was more the product of a statistical anomaly than a meaning point that defines vehicle emission performance. Staff also is concerned that the rational for the cutoff point of 0.6, applied specifically to NOx to produce an optimal statistical model, is not applicable to hydrocarbons and CO. The cutoff points that maximize the likelihood function for THC and CO are 1.0 and 1.6 times their tailpipe standard, respectively.

Staff also consulted with Dr. David Rocke of the University of California, Davis to provide comments and guidance regarding the validity of the Tech 4 NOx modeling approach proposed by the stakeholders. He concurred with staff that while the alternative approach might provide some improvement in statistical performance, other factors should be considered. In this case, it is essential that emissions modeling be consistent with sound engineering judgment and good science and have a sound basis relative to vehicle control system design and combustion chemistry. Relying on statistics as the sole guide to model construction could lead to misleading results. As a result, staff believes the suggested alternative is not appropriate and the approach taken to model Tech 4 vehicles in the previous Predictive Model modeling efforts should be maintained. This current approach was subject to independent scientific peer reviewed by appointees from the University of California in 1994 and 1999 and found to be reasonable and scientifically supportable."

It is important to point out that Staff and Dr. Rocke appear to agree (at least, they don't appear to disagree) that a dual model fits the Tech 4 data better than a single model. The major objections to utilizing the dual model appear to be:

- There are no physical response differences between vehicles emitting just below 0.6 times the NOx standard and those emitting just above 0.6 times the NOx standard,
- The alternative statistical method did not produce consistent results at the other pollutant cutpoints, and
- It is essential that emissions modeling be consistent with sound engineering judgment and good science and have a sound basis relative to vehicle control system design and combustion chemistry

The authors believe that the staff and the stakeholders in evaluating the dual model were overly focused on a very narrow aspect of the dual model – the engineering and combustion aspects of ethanol and NOx - and not enough focused on the fact that the dual model applies to all fuel parameters, and all pollutants, not just ethanol and NOx. The engineering and combustion factors for ethanol and NOx are complex. However, for other properties like sulfur and aromatics, it is relatively easy to demonstrate from an engineering standpoint why a dual model is better.

The authors of this paper agree with staff and Dr. Rocke that emission modeling must be consistent with sound engineering judgment, and that those developing this model must not rely on statistics alone to select sub-models for inclusion into the overall Predictive Model. But the authors of this paper believe that are good engineering reasons why the Tech 4 model performs better statistically than a single model. We present some of these reasons in this paper, and we invite comment on these reasons from others that are knowledgeable in this area.

Selecting the best model for Tech 4 vehicles is not merely an academic exercise with no impact on future fuels in California. Use of the dual model for Tech 4 vehicles could allow for increased flexibility for gasoline marketers in meeting the criteria of the Predictive Model, and may have a significant impact on the volume of ethanol used in the state, and other fuel parameters, when the model goes into effect. And, since the Predictive Model is also used by the staff estimating emission inventories to generate fuel correction factors for future versions of EMFAC, it is also critical that the model reflect the emissions of the entire fleet, so that emission inventories are more accurately estimated in California.

Some readers of this report may be wondering why we are proposing a change to the Tech 4 model, when there is no new Tech 4 data from the last model, and the Board approved the last two models with a single Tech 4 model. What has changed that compels a re-evaluation of this issue? In a word, it is the age of the Tech 4 fleet in the proposed Predictive Model calendar year of 2015 that requires reconsideration of this issue. The current model is based on 2005 – a full 10 years earlier than the proposed model. In 2015, the EMFAC2007 model predicts that the remaining Tech 4 fleet will have average odometer readings of about 225,000-250,000 miles. The EMFAC2007 model indicates that most of the emissions from the Tech 4 vehicles will be from higher emitters, even with the California vehicle emission inspection program. The average mileage of the Tech 4 fleet of test vehicles when it was tested was in the 15,000-25,000 mile range. Clearly, emission results developed 10-15 years ago on young vehicles are not directly applicable to a very old fleet.

Other readers may be wondering why we are not proposing a dual model for Tech 5 (1996+) vehicles. There are two primary reasons for this is – one is that the current Tech 5 database contains no higher emitters, and the second is that the manner in which the Tech 5 model is built, it does rely somewhat on the emission responses of higher emitting Tech 4 vehicles, so in a manner, it indirectly includes some higher emitting vehicles. A third reason is that the Tech 5 vehicles, with advanced emission controls and OBD, are not experiencing higher emitter frequencies like the earlier Tech 4 vehicles. Future fuels testing programs should probably evaluate higher mileage Tech 5 vehicles.

In this paper we examine the engineering and statistical reasons for a dual model, not just of NOx and ethanol, but for all Tech 4 fuel properties and exhaust pollutants. We also develop the dual model coefficients, the weighting factors, and create a fully functioning Predictive Model with a dual Tech 4 component that is identical in other respects to the proposed Predictive Model. The alternative model is complete in all respects and could

be viewed as a replacement for the single model. We also compare the two models and their responses to changes in fuel properties, and estimate the impact on future gasoline in California.

This paper is divided into the following sections:

- Section 3 – Background
- Section 4 - Importance of the Tech 4 Group in 2015
- Section 5 - Statistical Case for Dual Tech 4 Model
- Section 6 - Development of Tech 4 Dual Model Weighting Factors
- Section 7 - Implementation of Dual Tech 4 Model in Predictive Model
- Section 8 - Comparison of ARB Single Model and Dual Model, With Reasons for Differences

3. Background

This section discusses the Tech 4 model year group in the Predictive Model in more detail. It also references earlier work on Tech 4 vehicles showing differences in response between lower and higher emitters, and briefly discusses the EPA COMPLEX model, which is based on Tech 4 vehicles, and recognizes the different responses between lower and higher emitters.

3.1 Tech 4 vehicles

Tech 4 vehicles in the Predictive Model consist of test data on cars and LDTs (1s and 2s) in the 1986-2005 model years. The majority of vehicles are equipped with fuel injection – either throttle body injection (TBI) or multi-port fuel injection (MPFI), all have 3-way catalysts with a single oxygen sensor, and many have exhaust gas recirculation. Some Tech 4 vehicles were equipped with first generation onboard diagnostics (second generation OBD started in 1996).

Table 1 below shows the different EMFAC technology groups in the 1986-2005 model year range for Cars, LDT1s, LDT2s, and MDVs. We also show the population fraction for these technologies from this entire group of vehicles. The EMFAC tech groups should not be confused with the Predictive Model tech groups. The Tech 4 group in the Predictive Model includes only 1986-1995 model years, and therefore includes all EMFAC technology groups in those model years. There are many more technology groups in EMFAC than in the Predictive Model.

Table 1. EMFAC Technology Groups in Predictive Model Tech 4 Group Model Years

EMFAC Technology Group Number	2015 Population Percentage	Applicable Vehicle Class(es)	Technologies
10	10%	LDA/LDT/MDV	TWC. TBI/CARB, 0.7 NOx
13	19%	LDA/LDT/MDV	TWC, MPFI, 0.7 NOx
14	16%	LDA/LDT/MDV	TWC, TBI/CARB, 0.4 NOx
15	24%	LDA/LDT	TWC, MPFI, 0.4 NOx
17	5%	LDA/LDT	TWC, TBI/CARB, 0.25 HC (Tier 1)
18	20%	LDA/LDT	TWC, MPFI, 0.25 HC (Tier 1)
21	4%	LDA/LDT	Adv. TWC, MPFI, 0.25 HC
43	1%	LDA	Mexican Vehicle, 0.7 NOx
176	1%	LDA/LDT/MDV	Diesel
177	1%	LDA/LDT/MDV	Diesel

TWC = three way catalyst
TBI/CARB = either throttle body injection or carbureted fuel delivery
MPFI = multi-point fuel injection
Adv. TWC = advanced three way catalyst (higher cell density, improved washcoat)

The two diesel technology groups, 176 and 177, are not applicable to the Predictive Model.

3.2 Earlier Work on Tech 4 Lower vs Higher Emitters

A 1993 SAE paper discusses fuel effects on higher emitting Tech 4 vehicles. [2] Seven 1986 and 1987 high HC/CO emitting vehicles were studied with pairs of fuels representing different aromatics, olefins, RVP, sulfur, T90, ethanol, and MTBE levels. It is important to note that the vehicles were not selected for high NOx emissions, but for high HC or CO emissions, indicating that they were mostly running richly. One vehicle with high HC and CO also did have high NOx emissions, and that was likely due to malfunctioning EGR valve. Other vehicles experienced a variety of problems, including one vehicle that was found to have ignition system problems and another with an overly-wide injector pulse-width. The average catalytic conversion efficiencies of the higher emitters tested were 24%, 7%, and 40% for HC/CO, and NOx, while for normal emitters in an earlier testing program, conversion efficiencies were 86%, 76%, and 80%.

The testing showed that reducing aromatics and increasing ethanol (in separate tests) reduced HC emissions much more for higher emitters than for normal emitters. A similar, but less strong pattern was also shown for CO emissions. For NOx, reducing aromatics increased NOx more for higher emitters than for normal emitters, and increasing ethanol also increased NOx from higher emitters more than from normal emitters.

Both aromatics and ethanol were found to have an effect on the engine-out equivalence ratio, or EQR. [1] It is well known that 3-way catalytic converter efficiency at simultaneously reacting all 3 pollutants is greatest when the EQR is very close to 1.0. As the report indicates:

> "Fuel aromatics and oxygenates are the most important fuel variables in affecting emissions through EQR, These findings are not surprising because aromatics have a higher density and low hydrocarbon:carbon ratio and fuel oxygen has a direct effect on oxygen supply."

The report goes on to say:

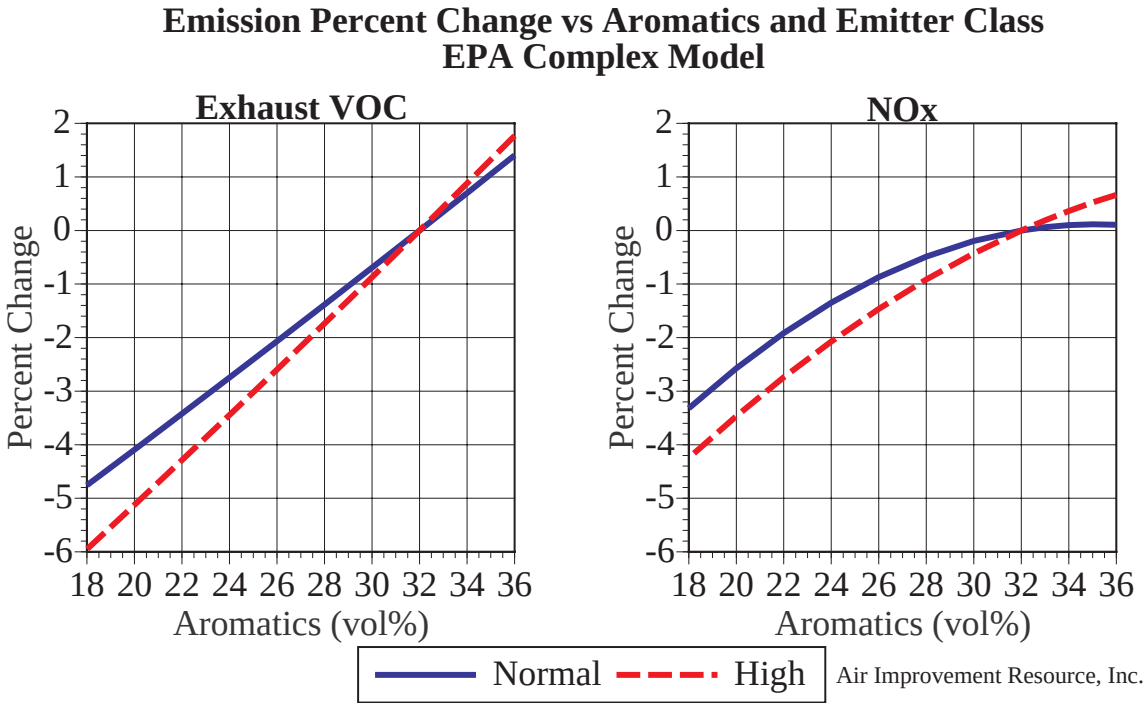
> "Reducing fuel sulfur and T90 may have less benefit on hydrocarbon emissions in these higher emitters than in normal emitters, and reducing sulfur may have less benefit on CO emissions. Reducing aromatics may be somewhat more helpful in reducing hydrocarbon and CO emissions in the high emitters.

Thus, this report gives credence to the idea that normal and higher emitters can experience different percent effects for changes in certain fuel parameters.

[1] EQR is a calculated value that compares the actual air;fuel ratio to the stoichiometric air:fuel ratio. EQR's less than 1 indicate that a vehicle is running rich, while EQRs greater than 1 indicate lean operation.

3.3 EPA COMPLEX Model

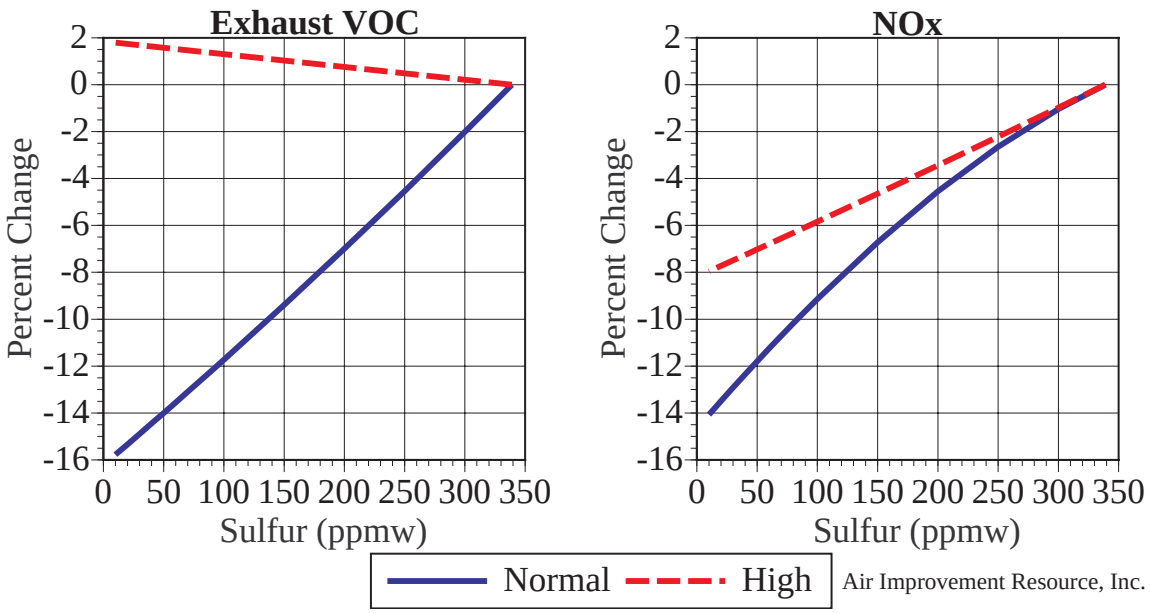
The EPA COMPLEX model, which was based on Tier 0 or Tech 4 vehicles, estimates emission responses of lower and higher emitting vehicles separately, and combines the two. AIR exercised this model for sulfur and aromatics as examples. The results are shown in the figures below.



For aromatics' effects on VOC and NOx, the COMPLEX model shows that higher emitters are more sensitive to aromatics than normal emitters. For sulfur effects on VOC and NOx, the COMPLEX model shows that higher emitters are much less sensitive to sulfur than normal emitters.

The COMPLEX model was developed over ten years ago, and used less data than we have now, and also used a much earlier version of the SAS program without the improvements that ARB uses today. We present these charts from the COMPLEX model not to suggest that this is how normal and higher emitters should be evaluated in the Predictive Model, but rather as additional evidence that other research has shown that there are differences in the way lower and higher emitters respond to fuel property changes.

Emission Percent Change vs Sulfur and Emitter Class
EPA Complex Model



4. Importance of Tech 4 Group in 2015

This section shows the importance of the Tech 4 group in calendar year 2015. Next, we determine the relative contributions of lower and higher emitter vehicles to Tech 4 emissions in 2015.

4.1 Tech 4 Group in 2015

As a first consideration, one has to ask the question: Why are Tech 4 vehicles important in 2015? They are between 20 and 30 years old, so there cannot be very many of them, and the ones that are out there may not be driven very much. So what is all the concern about whether they are modeled with a single model or a dual model?

Table 2 shows emissions weighting factors for the different technology groups in the latest Predictive Model, from Table 8 of the report. As shown in the table, the Tech 4 and Tech 5 (1996+) vehicles account for the majority of emissions. For example, Tech 4 and Tech 5 together account for 95% of the NOx and 92% of the THC. However, we were somewhat surprised that the Tech 4 vehicles account for 32.6% of the NOx emissions in calendar year 2015 (2015 is ARB's proposed calendar year for the Predictive Model), and 38% of the THC. Our examination of these vehicle groups for a statewide run of the EMFAC2007 model indicates that the Tech 4 vehicles only contribute 5.9% of the VMT from gasoline cars and light trucks in 2015.[2]

Table 2. Technology Weighting Factors in the Predictive Model

Pollutant	Tech 3	Tech 4	Tech 5
NOx	0.052	0.325	0.622
THC and Toxics	0.075	0.380	0.546
CO	0.063	0.288	0.649

Clearly, for the Tech 4 vehicles to contribute nearly 33-38% of the emissions while only contributing 5.9% of the VMT indicates that the model is predicting that the Tech 4 vehicles have much higher NOx emissions in 2015 per vehicle than the Tech 5 vehicles. There are two reasons for this: (1) the Tech 5 vehicles, which consist of LEV1s and LEV2s[3], are certified to much lower NOx standards than the Tech 4 vehicles, and (2) the Tech 4 vehicles that are still on the road in 2015 probably have quite high mileages, and have experienced deterioration in NOx emissions. But whatever the reasons, it is clear from the table that the Tech 4 group is still a very important group in how the Predictive Model predicts emissions from the fleet, even in calendar year 2015. Therefore, the method used to model emissions for this technology group should be carefully considered.

[2] Tech 5 vehicles contribute 93% of the vehicle miles traveled.

[3] LEV1s and LEV2s operating on gasoline can be TLEVs, LEVs, ULEVs, SULEVs, or PZEVs. The TLEV NOx full useful life NOx standard was 0.4 g/mi. The LEV1 and ULEV1 NOx full useful life NOx standard was 0.3 g/mi and the SULEV and PZEV NOx full useful life NOx standard is 0.01 g/mi. The LEV2 and ULEV2 NOx full useful life NOx standards were reduced further to 0.07 g/mi.

4.2 Comparison of Tested Tech 4 Vehicles vs Tech 4 Vehicles On-Road in 2015

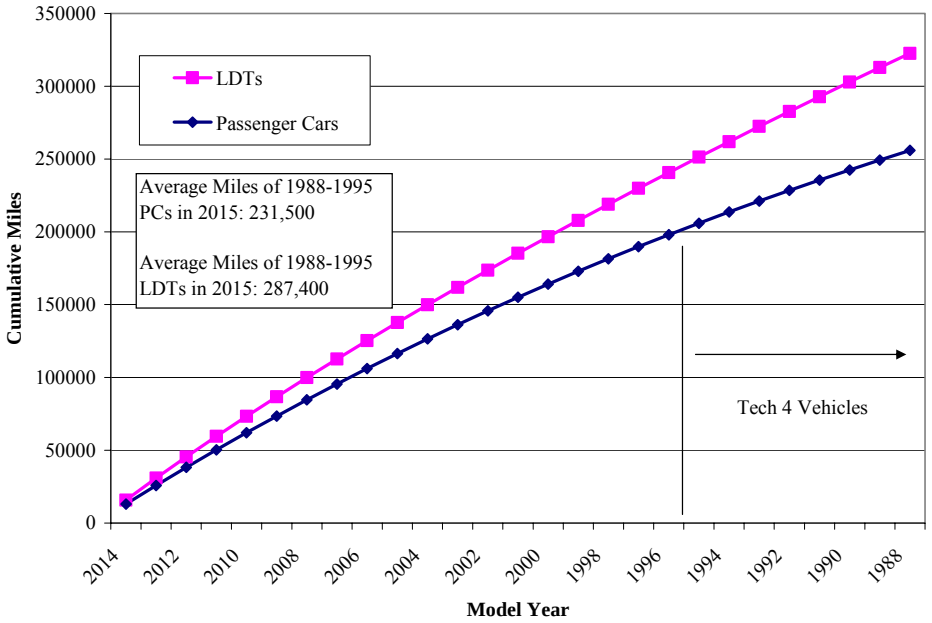
One of the most significant reasons for seriously considering the use of a dual model for Tech 4 vehicles, which considers potentially different responses for lower and higher emitters, is the age and emissions condition of the Tech 4 fleet in calendar year 2015, the calendar year of the new Predictive Model.

The Tech 4 vehicles used in the Predictive Model database were tested in the early 1990s. An analysis of the odometer readings of many of the vehicles tested in the Auto/Oil programs shows that when the vehicles first entered the program, they had between 15,000 miles and 20,000 miles. They then accumulated additional miles in the Auto/Oil testing program.

The first Predictive Model was released in 1995, and applied to California Phase 2 fuel, which was implemented in 1996. The first Predictive Model utilized a single model for Tech 4 vehicles, which was appropriate at that time because the mileage of the tested vehicles was similar to the mileage of the Tech 4 vehicles on the road. There were subsequent revisions to the Predictive Model, which also used a single model for Tech 4 vehicles. The last revision of the Predictive Model was in 1999.

With the passing of much time, however, the use of a single model for Tech 4 vehicles is much more questionable. The Tech 4 vehicles have accumulated much more mileage, and are much older than when the original Tech 4 vehicles were tested. As vehicles age, their emissions typically increase. The EMFAC2007 model estimates that Tech 4 passenger cars will have an average of about 231,000 miles and LDTs will have an average of 287,000 miles, as shown in the figure below. Of course, many Tech 4 vehicles will have been scrapped, but it is the vehicles remaining on the road that will have very high mileages and emissions.

Cumulative Miles of Tech 4 Vehicles in 2015
Source: EMFAC2007, South Coast Air Basin



The emissions of vehicles in EMFAC are estimated for different emitter regimes. The model also estimates growth in various emitter regimes with mileage. The overall emissions for a vehicle technology and model are estimated by combining the percentage of vehicles in each emitter regime with its average emissions.

Table 3 shows EMFAC2007's estimate of NOx emissions for 1991 model year vehicles in the Technology 15 group[4] for EMFAC2007 (MPFI, 3-way catalytic converter, 0.4 NOx). We show the fraction of this technology group in each emitter regime, the NOx emissions of the regime, and the contribution of each emitter regime to the total emissions. These estimates were made with EMFAC2007, assuming the California I/M program.

[4] The Tech 15 group in EMFAC2007 is a different tech group than the Tech 4 group in the Predictive Model. The Tech 15 group in EMFAC represents multi point fuel injected vehicles with 3-way catalytic converters, 1983-1994 model year group that meet a 0.4 NOx standard.

Table 3. Regime NOx Emission Rates of 1991 Model Year Tech 15 Vehicles in 2015 (I/M)					
Emitter Group	Multiple of Standard	Percent of 1991 fleet	NOx Emissions g/mi	Wtd Avg (Column 1* Column 2)	Percent of Emissions (Column 3 Normalized)
Normal	≤1x	30.0%	0.257	0.0773	14.3%
Moderate	>1-≤2x	63.1%	0.577	0.3639	67.8%
High	>2-≤5x	4.8%	0.993	0.0473	8.8%
Very High	>3-≤4x	0.7%	1.597	0.0107	2.0%
Super	>4x	1.4%	2.697	0.0377	7.1%

Results for this technology group in this model year in the 2015 calendar year show that less than 15% of the NOx emissions are from normal emitters (less than 1 times the NOx standard), and that the remaining 85% of emissions are from vehicles with NOx emissions more than the standard. Thus, by 2015, the Tech 4 fleet has changed considerably from the time the vehicles were originally tested, and it is inappropriate to apply fuel effects developed on a very young Tech 4 test fleet to a very old 2015 Tech 4 fleet, without taking into account the significant change in the emissions from higher versus lower NOx emitters.

Section 7 of this paper develops the fraction of emissions due to lower and higher emitters for all technologies in the Tech 4 groups for all three pollutants.

5. Tech 4 Technology, Higher Emitters, and Fuel Effects

In this section, first we discuss in more detail the Tech 4 technology and control systems. Next, we discuss why vehicles become higher emitters, and finally, we discuss general fuel composition changes on higher emitters.

5.1 Tech 4 Emission Control Technology

This is not a complete and detailed description of Tech 4 emission control technology, but it does provide enough information to enable the understanding of why certain fuel properties affect emissions more than others.

As indicated earlier, Tech 4 covers the 1986-1995 model years of passenger cars and LDTs. The Background section (Section 3) listed many of the technologies present in tech 4 vehicles, this section goes into more detail about these technologies and associated controls systems.

All of the Tech 4 vehicles were equipped with fuel injection, either throttle body injection (TBI) or multi-point fuel injection (MPFI). Exhaust emission controls included a 3-way catalytic converter, almost always underfloor and not close-coupled (these came later with the advent of the LEV and Tier 2 standards). The three-way catalyst is so named because it simultaneously reduces HC, CO, and NOx emissions. However, in order for the catalytic converter to have the highest reductions of all three pollutants, the air fuel ratio to the engine and catalyst must be maintained very close to stoichiometric conditions.

Maintenance of the air/fuel ratio close to stoichiometric conditions is assisted by an oxygen sensor placed in the exhaust system ahead of the catalyst. If there is too much oxygen in the exhaust stream ahead of the catalyst, the oxygen sensor and onboard computer working in conjunction with other sensors command less air, more fuel, or both. If there is not enough oxygen in the exhaust stream, then opposite adjustments are made. Other sensors were also used in commanding air fuel ratio, such as and manifold absolute pressure sensor (MAP), coolant temperature sensor, air temperature sensor, and so on.

So called “closed loop” feedback engine control systems utilized in Tech 4 vehicles operate in the “open loop” mode during cold start, before the catalytic converter is warmed up. This means that they use cold start enrichment and pre-programmed fueling strategies that ensure good drivability and quick catalyst warm-up. Current vehicles meeting more stringent standards must use aggressive cold start and warm-up control strategies such as close-coupled converters that reach the operating temperature very quickly, and stoichiometric air/fuel ratio.

Air/fuel ratio control in Tech 4 vehicles is good, but not nearly as precise as in today’s vehicles. Today’s vehicles employ two oxygen sensors, one ahead of the catalyst and one

behind. The second oxygen sensor is used to "trim" control to ensure very tight control of air/fuel ratio at all times to maximize catalyst efficiency for oxidation of HC and CO and reduction of NOx.

More stringent emission standards and new durability requirements drove several fundamental control system design changes in Tech 5 vehicles. While catalyst efficiencies in Tech 4 vehicles were in the range of 60 to 80% for NOx and 70 to 90% for HC and CO, Tech 5 designs relied on much higher efficiencies in the range of 95 to 99% after catalyst warm-up. Higher catalyst efficiencies and improved catalyst designs in many cases permitted the elimination of less reliable components such as secondary air systems and EGR found on Tech 4 vehicles. Much more precise air-fuel ratio control was also required to maintain these high efficiencies for extended useful like intervals to 100,000 miles. Strategies were employed to dramatically reduce catalyst warm-up time, and sophisticated predictive algorithms were developed for cold start and open loop operation.

On-Board Diagnostic (OBD) regulations were first required by California in 1991 model year light duty vehicles. This was a very limited pilot application of the complex and sophisticated ODB systems that were required nationally beginning with 1996 Tech 5 vehicles. The application of OBD II in 1996 and later resulted in major improvements in in-use emissions performance. It forced the design of more durable control systems and more reliable components such as valves and switches. The OBD malfunction indicator light also encouraged consumers to seek repairs of malfunctioning systems. More reliable emission control system design in Tech 5 vehicles has resulted in far fewer higher emitter vehicles compared to the Tech 4 fleet. Fundamental emission control system design differences driven by more stringent emission standards and OBD requirement has resulted in different in-use emission characteristics of Tech 5 vehicles compared to Tech 4.

Tech 4 vehicles also employ an open loop strategy and rich fueling during high acceleration and high load conditions (for example, towing for LDTs). The purpose of this rich operation is to ensure that the catalytic converter does not overheat, thereby lowering its performance. Rich operation during high acceleration modes was significantly reduced with the implementation of the Supplemental Federal Test Procedure requirements that started with model year 2000 passenger cars.

Many Tech 4 vehicles are also equipped with exhaust gas recirculation (EGR) to reduce NOx emissions.

5.2 General Causes of High Emissions in Tech 4 Vehicles

Vehicles can become higher emitters in one of four general ways. In the first way the oxygen sensor or one of the other sensors that feed data to the ECU malfunctions, and the system does not properly sense the air fuel ratio coming to catalytic converter, or the vehicle goes into permanent open loop mode. These are the kind of "rich" failures that usually result in higher HC and CO emissions, and lower NOx. In many cases, there is

nothing wrong with the catalytic converter, but it is not able to operate at its designed efficiency because the proper air fuel ratio coming to the converter cannot be maintained.

The second kind of higher emitter is where the catalytic converter deteriorates, losing its efficiency. In this case, the air fuel ratio control system can be operating properly, but the converter has lost some of its effectives. This can occur if the converter has for some reason been operated in a high temperature condition, or if deposits from the gasoline or oil have coated the catalyst (for example, if oil consumption has increased), rendering it less effective. If the catalyst has lost much of its efficiency, then not only do HC and CO emissions increase, but NOx increases also.

The third way is a combination of the first two ways – the vehicle loses air/fuel ratio control, and the catalyst performance is also low. This results in high HC, CO, and NOx emissions.

In the fourth way, the EGR system can also malfunction or become plugged, resulting in increased NOx emissions.

Of course, the California I/M biennial and change-of-ownership program can help find these vehicles, and cause them to be repaired. However, many vehicles can fail and operate a long time before their next inspection. In addition, unregistered vehicles that are also higher emitters are able to circumvent the I/M program. As indicated earlier in this section, the ARB EMFAC2007 model indicates that most of the emissions from Tech 4 vehicles are from higher emitters, even with the California I/M program in place.

5.3 Comparison of How Fuel Properties Can Affect Lower and Higher Emitters

Generally, Tech 4 normal emitters have relatively high cold start emissions (before the catalytic converter is "warmed-up"), and very low warmed-up emissions. Higher emitters will have high cold start emissions, but will typically also have high warmed-up emissions as well. This is a key difference that is a major cause of differences between low and higher emitters in terms of fuel effects.

5.3.1 Distillation Properties

Distillation properties such as RVP, T50 and T90 typically affect cold start emissions before the engine is fully warmed up. In a cold engine, if the fuel is not burned well, then HC emissions will be high. In normal emitting vehicles, then, distillation properties will really only have a significant affect on the cold start emissions, and once the engine and catalyst are fully warmed up, distillation properties do not have much of an effect. The same is true for higher emitters – distillation properties affect how the engine starts and runs before the engine is warm. But since total emissions from higher emitters is much higher because either air:fuel ratio control is bad during warm vehicle operation or the catalyst is compromised, or both, then the percent effect of distillation properties in higher emitters should be less than in normal or lower emitters.

5.3.2 Sulfur

One of the best examples of the differences in fuel property effects between lower and higher emitters is sulfur. Sulfur does not affect engine-out HC, CO, or NOx emissions at all, but it does affect catalyst efficiency (sulfur does affect engine-out SO_2 emissions and tailpipe sulfate PM emissions).

In a normal emitting Tech 4 vehicle, increased sulfur levels will reduce catalyst efficiency, leading to increases in HC, CO and NOx. However, a higher emitting vehicle with a very low efficiency or zero efficiency catalyst will experience no increase in HC, CO, and NOx emissions because the catalyst efficiency is already so low it can hardly be impacted. Thus, with sulfur, there is a clear difference in the percent change in emissions between lower and higher emitting vehicles due to sulfur levels.

5.3.3 Aromatics

As indicated in the background section and SAE 930137, aromatics have a higher carbon to hydrogen ratio, and cause the oxygen to be depleted in the exhaust stream. In normal emitting vehicles with good air:fuel ratio control, the oxygen sensor and 3-way catalyst can mostly compensate for this. However, in higher emitters with poor air:fuel ratio control, or vehicles with severely compromised catalytic converters, the 3-way system is unable to compensate. Therefore, increasing aromatics has a greater percentage effect at increasing HC emissions on higher emitters than on lower emitters.

5.3.4 Oxygen – Ethanol

Ethanol's effects on emissions are complex. First, ethanol reduces engine-out HC, CO, and NOx emissions. Ethanol causes a slight enleanment effect in the exhaust stream. The extra oxygen in the exhaust stream reacts some of the unburned HC and CO in the exhaust stream. However, engine-out NOx emissions are also reduced because ethanol's higher heat of vaporization lowers flame temperatures during combustion. [3]

While ethanol reduces engine-out HC, CO, and NOx, it also causes an enleanment in the air fuel ratio coming to catalyst (the opposite of aromatics). This lean shift reduces NOx conversion efficiency, causing an increase in NOx.

The change in behavior between lower and higher NOx emitters is consistent with a slightly lean shift in the engine with ethanol, and the change in NOx conversion efficiency in the catalyst. Tech 4 vehicles typically had engine out NOx levels of 0.5-2.2 g/mi, and utilized catalytic converters with average efficiencies of 60-80%. Modern Tech 5 vehicles must have NOx conversion efficiencies of 95-99% in order to meet the lower NOx standards.

A lower emitting Tech 4 vehicle, i.e., one below 0.6 g/mi, would probably have a NOx conversion efficiency of 80% or more. A higher emitting Tech 4 vehicle with some loss of converter efficiency could be in the 40% range. The use of ethanol in both vehicles could cause a small converter efficiency loss in both converters due to lean shifts during

acceleration events where NOx is produced. A fixed efficiency loss would cause a greater percent increase in NOx in the 80% efficient catalyst than in the 40% efficient catalyst. The percent increase in emissions for these two catalysts, assuming both a 2% loss in catalyst efficiency, is shown in Table 4.

Table 4. Theoretical Change in NOx for a Lower and Higher Emitting Vehicle Due to Small Catalyst Efficiency Loss

Emitter	Engine-Out NOx g/mi	Catalyst Efficiency	Tailpipe g/mi	Catalyst Efficiency Loss due to ETOH	Tailpipe with ETOH	% Increase in NOx
Lower	2.0	80%	0.4	2%	0.44	10.0%
Higher	2.0	40%	1.2	2%	1.24	3.3%

The table shows that a 2% loss in catalyst NOx efficiency could cause a 10% increase in NOx in the vehicle with a 80% conversion efficiency, and a much lower 3% increase in NOx in the vehicle with a 40% conversion efficiency.

If this is the mechanism, then we would expect to see less of a percent increase in NOx for higher emitters than lower emitters. We divided all Tech 4 vehicles into 3 emitter groups, 0-0.6 g/mi, 0.601-1.0 g/mi, and 1.001+ g/mi, and then fit the latest ARB mixed model through the NOx data for each emitter group, and then estimated the percent increase in NOx from 2.0 wt% to 3.5%. The results are shown in Table 5.

Table 5. Comparison of NOx Responses of Different Emitter Groups

Group	# Vehicles	# Vehicle/Fuel Combinations	% Increase in NOx from 2.0 to 3.5 wt %
0-0.6 g/mi	537	2359	8.6%
0.601-1.0 g/mi	242	1176	3.0%
1.001+ g/mi	121	650	0.35%

The results show a declining sensitivity to ethanol with increasing NOx emissions, such that vehicles over about 1.00 g/mi do not appear to experience an increase in NOx.

5.3.5 Summary of Fuel Impacts

The previous discussion show that certain fuel properties- most notably distillation properties such as T50 and T90 ,sulfur, aromatics, and ethanol – should be *expected* to have different percent effects on lower and higher emitters. And, since most of the emissions from the Tech 4 fleet in 2015 are from higher emitters, it is very important that lower and higher emitting vehicles be modeled separately.

6. Statistical Case for Dual Tech 4 Model

6.1 Comparison of Statistics of Dual and Single Models

The ARB single model for Tech 4 assumes that all Tech 4 vehicles have the same distribution of emissions responses to changes in the fuel parameters. The dual model approach allows for the possibility that lower-emitting vehicles respond differently than higher emitters. Obviously the lower emitters have lower vehicle average emissions, but the dual model implies that the vehicle average percentage changes in emissions due to changes in fuels are different for the lower and higher emitters. The dual model uses exactly the same statistical model as the single model but is fit separately to the lower and higher emitter subsets. The dual model fits the Tech 4 data statistically significantly better than the single model, as shown in the following.

To define the dual model for each pollutant, NOx, THC, CO, the emissions level for each tested vehicle were defined as the average emissions on Auto/Oil fuel A. If the vehicle was not tested on Auto/Oil fuel A, then the vehicle's nearest test fuel to fuel A was used, based on the normalized Euclidean distance between the seven fuel parameters. Thus we take each squared difference between the test fuel parameter and the fuel parameter for Auto/Oil fuel A and divide the squared difference by the fuel parameter variance. We then find the test fuel such that the sum of these seven normalized differences is smallest. For a given emissions cutoff, the lower emitters are vehicles emitting below the cutoff and the higher emitters are vehicles emitting more than the cutoff. The dual model results are not very sensitive to the definition of the vehicle's emissions level because the variability between emissions on different vehicles is generally much greater than the variability between emissions on the same vehicle using different fuels.

To find the best-fitting dual model, a range of emission cutoffs were considered. The ARB splits vehicles into different emitter regimes, and the definition of these regimes are shown in Table 6.

Table 6. Emission Regimes as a Multiple of the Emission Standard (EMFAC2002 and EMFAC2007)

Regime	HC	CO	NOx
Normal	<1x	<1x	<1x
Moderate	1x-2x	1x-2x	1x-2x
High	2x-3x	2x-3x	2x-3x
Very High	3x-4x	3x-4x	3x-4x
Super	>4x	>4x	>4x

The regimes are defined as multiples of the applicable emission standards. Therefore, for Tech 4 vehicles with a NOx standard of 1.0 g/mi (50,000 miles), normal emitters are considered all that are below 1.0 g/mi.

The ARB defined the regimes in this way across many different vehicle types and model years. The definitions were not evaluated statistically, i.e., they do not represent any fixed

percentiles of the emissions data. They are based on the emission standards, and that makes sense because vehicles emitting above their emission standards could be considered "higher emitters." New vehicles typically emit below their standards, so a vehicle emitting above its standard could be considered a "high emitter." The definitions are really just a method of splitting the data, and then developing the rate of growth of vehicles in the higher emitting categories. They could have been split at multiples of 1.5 times the various standards instead of 1x the standard for example, the regime growth rates could have been estimated, and the EMFAC model would estimate the same overall emissions. In other words, the regime definitions are closely allied to the regime growth rates, and that is all that matters in using this process to evaluate emissions as the fleet of vehicles ages.

For our purposes, however, we do not want to merely use the EMFAC definitions of a lower and higher emitter. This is best left to an analysis of the data. A number of different lower vs. higher emitter "cutoffs" should be evaluated, and we should pick the one with the best "fit." If this coincides with the cutoffs displayed in Table 3, then that is acceptable. But we would be quite surprised if the lower versus higher emitter cutoff values as determined by the best fit of the data indicated that it was at 1x of all three of the emission standards.

The relevant emissions standards for Tech 4 vehicles are 1 g/mi NOx, 0.41 g/mi THC, and 3.4 g/mi CO. In each case we considered cutoffs of 20%, 30%, …, 200% of the applicable standard (only the cutoffs closest to the ideal cutoffs are shown in the table). The best-fitting model is the model with the highest likelihood, which is the probability density of the fitted dual model. The likelihood is a standard measure of the goodness-of-fit of a statistical model. However, its value depends upon the number of observations and the variability in the data, so it is not a meaningful number by itself and can only be used to compare different statistical models on the same data set. Taking logarithms, the best-fitting dual model is the one with the lowest value of "-2*log-likelihood." The results of this analysis are shown in Table 7. Each model was fitted using the method of maximum likelihood. The values of -2*log-likelihood for each pollutant and cutoff are given in the third column. The best-fitting dual models (i.e., with the lowest -2*log-likelihood) are highlighted in yellow: 160 % of the standard (5.44 g/mi) for CO, 60 % of the standard (0.6 g/mi) for NOx, and 100 % of the standard (0.41 g/mi) for THC. These best fitting dual models fit the data better than either of the single models shown.

Table 7. Log-likelihood and P-values for Different Dual Models					
		-2*Log Likelihood			
Pollutant	Percentage Cutoff	Dual	Single Same Vehicle Intercept	Single Diff Vehicle Intercept	P-value Fuel Effects
CO	20	447.83	552.18	502.71	5.10E-04
	30	365.91	552.18	417.33	1.42E-03
	40	133.36	552.18	186.68	8.14E-04
	50	-49.76	552.18	13.05	4.25E-05
	60	-154.04	552.18	-79.68	8.51E-07
	70	-237.30	552.18	-177.05	9.66E-05
	80	-284.88	552.18	-226.18	1.57E-04
	90	-345.93	552.18	-287.49	1.71E-04
	100	-385.12	552.18	-318.14	1.07E-05
	110	-403.85	552.18	-339.68	2.72E-05
	120	-419.82	552.18	-350.68	5.16E-06
	130	-427.09	552.18	-344.96	5.26E-08
	140	-427.74	552.18	-337.63	2.75E-09
	150	-443.18	552.18	-340.95	2.64E-11
	160	-448.12	552.18	-326.09	9.66E-15
	170	-444.74	552.18	-325.04	2.50E-14
	180	-429.71	552.18	-320.30	1.56E-12
	190	-434.88	552.18	-313.04	1.04E-14
	200	-434.29	552.18	-311.52	7.11E-15
NOx	20	-2846.55	-2459.87	-2806.64	5.22E-02
	30	-3067.89	-2459.87	-3006.25	1.60E-04
	40	-3275.09	-2459.87	-3147.49	5.22E-15
	50	-3295.29	-2459.87	-3164.42	1.33E-15
	60	-3345.24	-2459.87	-3139.17	0.00E+00
	70	-3317.49	-2459.87	-3098.13	0.00E+00
	80	-3208.16	-2459.87	-3023.32	0.00E+00
	90	-3145.39	-2459.87	-2958.77	0.00E+00
	100	-3083.71	-2459.87	-2904.53	0.00E+00
	110	-3016.05	-2459.87	-2844.14	0.00E+00
	120	-2979.99	-2459.87	-2819.56	0.00E+00
	130	-2959.84	-2459.87	-2795.10	0.00E+00
	140	-2952.79	-2459.87	-2779.90	0.00E+00
	150	-2918.58	-2459.87	-2760.32	0.00E+00
	160	-2942.62	-2459.87	-2750.34	0.00E+00
	170	-2929.05	-2459.87	-2743.43	0.00E+00
	180	-2915.88	-2459.87	-2733.21	0.00E+00
	190	-2877.69	-2459.87	-2711.53	0.00E+00
	200	-2833.84	-2459.87	-2689.87	0.00E+00
THC	20	-1333.51	-1257.28	-1291.56	9.06E-02
	30	-1474.86	-1257.28	-1428.26	3.57E-02
	40	-1876.69	-1257.28	-1765.28	5.32E-11

Table 7. Log-likelihood and P-values for Different Dual Models					
Pollutant	Percentage Cutoff	-2*Log Likelihood			P-value Fuel Effects
		Dual	Single Same Vehicle Intercept	Single Diff Vehicle Intercept	
	50	-2201.28	-1257.28	-2034.26	0.00E+00
	60	-2280.97	-1257.28	-2180.14	2.57E-09
	70	-2350.74	-1257.28	-2265.52	5.92E-07
	80	-2388.64	-1257.28	-2290.99	8.02E-09
	90	-2445.16	-1257.28	-2308.14	2.78E-15
	100	-2449.47	-1257.28	-2299.57	0.00E+00
	110	-2437.40	-1257.28	-2268.29	0.00E+00
	120	-2437.67	-1257.28	-2256.90	0.00E+00
	130	-2396.10	-1257.28	-2211.51	0.00E+00
	140	-2396.86	-1257.28	-2198.14	0.00E+00
	150	-2285.40	-1257.28	-2167.42	4.50E-12
	160	-2281.07	-1257.28	-2148.06	1.34E-14
	170	-2260.12	-1257.28	-2124.91	5.66E-15
	180	-2243.66	-1257.28	-2085.09	0.00E+00
	190	-2217.17	-1257.28	-2060.92	0.00E+00
	200	-2200.10	-1257.28	-2040.74	0.00E+00

The fourth column ("Single Same Vehicle Intercept") in Table 1 gives -2*log-likelihood for the ARB single model (fitted by maximum likelihood). Obviously the dual model fits better since it has lower values of -2*log-likelihood, but the statistical test evaluates whether the improvement is attributable to random variation, since the dual model has many more parameters to be fitted. It is not very meaningful to directly compare the dual and single models, because the dual model has different average vehicle intercepts as well as different average fuel coefficients; we are interested in whether the higher emitters respond differently to fuel changes and not the obvious fact that the higher emitters have a higher average emissions. Therefore we compare the dual model with a version of the single model that fits a different intercept but the same fuel coefficients for the higher and lower emitters. This tests whether lower and higher emitters respond differently to fuel changes. The values of -2*log-likelihood for this adjusted single model are shown in the fifth column ("Single Diff Veh Intercept"). The likelihood ratio test uses the difference between the values of -2*log-likelihood for the dual and adjusted single models. For example, for the dual NOx model with a cutoff of 60 %, the difference is 3345 - 3139 = 206. If the lower and higher emitters respond the same way, then the difference approximately has a chi-square distribution (the degrees of freedom is the number of extra parameters in the dual model).

The likelihood ratio test uses the difference between the values of -2*log-likelihood for the dual and adjusted single models. For example, for the dual NOx model with a cutoff of 60 %, the difference is 3345 - 3139 = 206. If the lower and higher emitters respond the same way, then the difference approximately has a chi-square distribution (the degrees of freedom is the number of extra parameters in the dual model). Therefore, if the observed

difference exceeds the 95th percentile of the chi-square distribution, then we can infer that the difference in observed responses for lower and higher emitters is not due to chance and we reject the hypothesis that the lower and higher emitters respond the same way (at the 5 percent level). This is mathematically the same as defining the p-value as the probability that the chi-square exceeds D, the observed difference, and then inferring that the lower and higher emitters respond statistically significantly differently whenever the p-value is less than 5 % (for a test at the 5 percent significance level). The p-values are shown in the final column. (For example, for the dual NOx model with a cutoff of 60 %, the difference 206 is compared to a chi-square distribution with 27 degrees of freedom, and has a p-value of 0.000 to the available precision of the statistical software). These are the probabilities of getting these differences by chance. For the best-fitting dual models the p-values are all less than 10^{-15}. Thus the dual models fit the data statistically significantly better than either of the single models, at an extreme level of significance.

Concerns have been raised that the p-values may not be accurately estimated by these procedures. Some reasons why these calculations may be inaccurate are:

- The chi-square distribution for the likelihood ratio test is an approximation for large samples.

- The asymptotics may not apply in cases where the estimated parameter values are on the boundary of the parameter space (in this case, some of the estimated covariance parameters are zero).

- The emissions data are used twice, to subdivide vehicles into lower and higher emitters and again to fit the separate lower and higher emitter models.

- The selection of the optimal cut-off based on finding the fitted dual model with the highest log-likelihood may impact the distribution of the test statistic.

To address these concerns, a bootstrap procedure was applied to confirm the p-values for the case of the NOx dual model with a 0.6 g/mi cutoff. The details are given in Attachment 1. The results of the 1096 simulations showed that the p-value is no more than 1/1096, but would be expected to be much lower than that. Thus, even if the assumptions and approximations used to develop the p-values in Table 7 are not valid, this much more exact analysis still shows that for NOx at 60 %, the lower and higher emitters respond statistically significantly differently, at the usual significance level of 5 % and also at more extreme significance levels of below 0.1 %. It is reasonable to assume that we would get similar results for the other cutoffs and other pollutants.

A couple of additional statistical issues have been raised. First, the estimated coefficients may be biased because the emissions data are used twice, to subdivide vehicles into lower and higher emitters and again to fit the separate lower and higher emitter models. This issue is addressed by fitting an alternative model based on the difference in emissions between the test fuel and fuel A. The alternative model is not subject to this potential bias

and the estimated predictive model coefficients were very similar to those of the above dual models. For more details, see Attachment 2.

A second statistical issue concerns the discontinuity of the dual model. For a given cut-off, the dual model implies that a vehicle with emissions just below the cut-off has a very different emissions response to fuel changes than a vehicle with slightly higher emissions just above the cut-off. The discontinuity in response would not be expected for real world emissions.

To answer this point, we note that this phenomenon only occurs for a few vehicles on the borderline. A more realistic, continuous model approach might be to assume that vehicles with emissions below the cut-off minus some small amount respond to fuel changes according to the lower emitter model, that vehicles with emissions above the cut-off plus some small amount respond to fuel changes according to the higher emitter model, and that the response function for vehicles within a small amount of the cut-off varies continuously from the lower emitter response function to the higher emitter response function. For the bulk of the test fleet and the on-road fleet, the emissions on a given vehicle will remain on one side or other of the cut-off because the variability in emissions from test-to-test or fuel-to-fuel is much smaller than the variability from vehicle to vehicle. Therefore, for the bulk of the fleets, the percentage changes in emissions will be correctly estimated by the lower or higher emitter models, but the percentage changes will be incorrectly estimated for a few vehicles on the borderline. Thus the potential error in the estimated fleet percentage changes due to wrongly assuming a discontinuous response for vehicles on the borderline is negligible. In this regard, the dual model is no less realistic than the EMFAC model itself, which also groups vehicles into ranges according to their emissions levels. Finally, we note that when the lower and higher emitter group emissions are weighted together in the model (see Sections 7 and 8), there is no discontinuity in the emissions prediction of the weighted average emissions as the fuel properties are varied.

Another more general way to address the discontinuity issue is to consider that the dual model is a simple approximation to a continuous model where the response function varies continuously with the emissions level. (The continuous model described in the last paragraph is a special case of this). In other words, instead of a dual model with only two groups of vehicles, we could imagine a hypothetical limiting case of a continuous model with infinitely many groups. The dual model is a simple approximation to this infinite group model. If more data were available, it would be possible to subdivide the Tech 4 emissions data into more than two groups and thus get closer to the true infinite group model. However, since each additional group increases the model complexity (a concern expressed by Dr. Rocke) and also increases the uncertainty of the estimated parameters, keeping the number of groups to only 2 seems to be warranted.

In summary, the statistical tests show that the dual models for NOx, THC, and CO each fit the Tech 4 data statistically significantly better than the single models. We can be at least 99.9 % confident that the higher emitters respond to fuel changes differently to the lower emitters.

6.2 Dual Model Coefficients

The dual model coefficients developed using the methods described above are found in the following tables. A comparison of the dual and single models is shown in Section 8.

Table 8. NOx Dual Model Coefficients		
Effect	≤60% Standard	>60% Standard
Intercept	-1.036582034	-0.053146215
RV	0.011106481	0.001303122
T5	-0.002709548	0.000888682
T9	0.003844741	-0.001726558
AR	0.015049225	0.014313734
OL	0.015758869	0.01681794
OX	0.020802624	0.005389046
SU	0.059252001	0.023587033
T5T5	0.008104656	0.003222909
T9AR	-0.004149611	-0.00154789
SUOX	-0.014106108	-0.008537121
ARSU	0.009936511	-0.00023821
OXOX	0.017354857	0.005759989
SUSU	-0.002758489	-0.00512299

Table 9. THC Dual Model Coefficients		
Effect	≤100% Standard	>100% Standard
Intercept	-1.579211083	-0.217275171
RV	0.020588309	-0.004173268
T5	0.059239382	0.047417581
T9	0.027348947	0.029103327
AR	0.001112741	-0.005972808
OL	-0.00928253	-0.013082313
OX	-0.009087462	-0.043034238
SU	0.06213948	0.043328686
T5AR	0.016710559	0.044403294
T5T5	0.016932876	0.011567171
T5OX	0.012801839	-0.000364608
T9T9	0.015049847	0.014141717
ARAR	-0.009003853	-0.026344995
AROX	0.005027605	0.027691067
SUSU	-0.00890793	-0.005455507
T9SU	-0.009130698	-0.002898858

Table 10. CO Dual Model Coefficients		
Effect	≤160% Standard	>160% Standard
Intercept	0.840969606	2.450589972
RV	0.026396627	-0.007368889
T5	0.024899662	0.020127308
T9	-0.009705268	-0.000185004
AR	0.025776721	0.034131705
OL	0.00438111	-0.006803501
OX	-0.04263169	-0.088033818
SU	0.057737641	0.046988618
SUSU	-0.006969771	-0.008246927
OXOX	-0.015611744	-0.007393381
T5AR	0.008783788	0.03095925
T9OL	-0.007630542	-0.006238788
T9T9	0.007320487	0.008464091

7. Development of Tech 4 Dual Model Weighting Factors

The weighting factors for the different technologies were shown in Table 1. Tech 4 vehicles contribute 33 percent of the NOx, 38 percent of the THC, and 29 percent of the CO. With the dual model, we must estimate the fraction of each of these percentages due to vehicles above and below the lower and higher emitter cutpoints of 60% of the standard for NOx, 160 percent of the standard for CO, and 100 percent of the standard for THC.

These fractions must be developed through EMFAC2007 modeling in order to include all of the technology groups that are represented by the Tech 4 vehicles, and also to utilize ambient temperatures, humidities, vehicle speeds, and all other variables that go into estimating emissions in California. This modeling takes advantage of the manner in which emissions are estimated for the different regimes.

For HC, since the cutpoint is 100% of the standard, this cutoff corresponds exactly to the normal emitters, that is, the normal emitters represent those vehicles at the standard and below, and all other emitter groups (moderates, highs, very highs and supers) represent all emitter groups above 100 percent of the standard. With this situation, it is possible to recode the model to produce emissions from 100 percent normal emitters, and then reprogram the model to produce emissions from 100 percent non-normal emitters. Then, the normal emitter fraction is represented by the following expression:

All Emitters = A * (Standard) + (1-A) * (Non-Normals)

Where

All emitters = emissions directly from EMFAC2007
A = fraction of Tech 4 emissions due to normals
Standard = emissions from running EMFAC only for normals
Non-normals = emissions from running EMFAC just for the non-normals

An example of this estimate for THC (statewide) follows:

All emitters, 2015: 38.8 tpd
Just normals, 2015: 16.4 tpd
Just non-normals, 2015: 43 tpd

38.8 = A*16.4 + (1-A)*43
A = 0.16

Thus, just 16% of exhaust THC emissions from the 1986-1995 fleet in 2015 is from normals, and 84% is from non-normals.

For NOx and CO however, the cutpoints do not match the emitter groups. For NOx, the optimum cutpoint splits the normal emitters, and for CO, the optimum cutpoint splits the

moderate emitters. To estimate the fractions for CO and NOx, we ran the EMFAC model at 200 percent of each standard (splitting the regimes into normals + moderates vs. highs + very highs + supers), and again at 100 percent of the standard (normals vs. moderates + highs + very highs + supers), and developed the lower vs. higher emitter fractions at 100 percent of the standards and 200 percent of the standards, similar to HC. Then, we developed the CO fractions at 160 percent of the standard by linear interpolation between 200 percent and 100 percent, and estimated the NOx low and high emitter fractions by extrapolating from the 200 percent and 100 percent fractions. While we are not sure that the process is linear between these cutpoints, we believe this is a reasonable approximation of the lower vs. higher emitter fractions at these cutpoints. The final low and higher emitter fractions for Tech 4 vehicles are shown in Table 11. Detailed calculations for this procedure are shown in Attachment 3.

Table 11. Tech 4 Lower and Higher Emitter Weighting Factors

Pollutant	Standard Factor	Lower Emitter Weighting Factor	Higher Emitter Weighting Factor
TOG- Exhaust	1.0	0.155	0.845
TOG - Evap	1.0	0.438	0.562
TOG – Total	1.0	0.377	0.623
CO	1.6	0.732	0.268
NOx	0.6	0.309	0.691

8. Implementation of Dual Model in Predictive Model

The Tech 4 dual model can be readily implemented in the current Predictive Model simply by inputting the dual model coefficients in the model, estimating the separate lower and higher emissions within the model, and weighting these emissions together using the weighting factors presented in the previous section. AIR did this, and we present a comparison of the results of the dual model versus the single model in the following section.

However, there is one issue that must be considered when doing the above. The Tech 5 model is constructed utilizing all of the Tech 4 vehicles as well, and this is described very well in the ISOR and will not be repeated here. If a dual Tech 4 model is used, and we believe it must be used, there are actually two choices for the construction of the Tech 5 model, as follows:

1. It can be built using all of the Tech 4 and Tech 5 vehicles (current Tech 5 model)
2. It can be built using just the "normal" Tech 4 vehicles and all of the Tech 5 vehicles

As indicated earlier, there are no higher emitters among the Tech 5 vehicles. The primary reasons for this are (1) that many Tech 5 vehicles of interest (mainly LEV1 and LEV2 vehicles) are only now starting to accumulate enough in-use mileage that some of them may be higher emitters, (2) the frequency of failure of these vehicles is much lower than earlier Tech 4 vehicles, and (3) there was a desire on the part of the testing community to determine the effects of fuel parameters on properly operating vehicles of new technology first.

Our recommendation is Option 1, and that is what we have followed in the remainder of this report. Option 1 makes the assumption that some of the Tech 5 vehicles will become higher emitters eventually.

9. Comparison of ARB Single Model and Dual Model

In this section, first we compare the dual model against the ARB single model for the primary properties for which there are significant differences – aromatics, oxygen, sulfur, T50, and T90 (the differences for sulfur are small, but we include them anyway). A complete set of comparisons for the all properties are presented in Attachment 4. Next, we use the dual model to estimate the change in ozone forming potential and NOx for the four sample fuels presented by ARB in the ISOR.

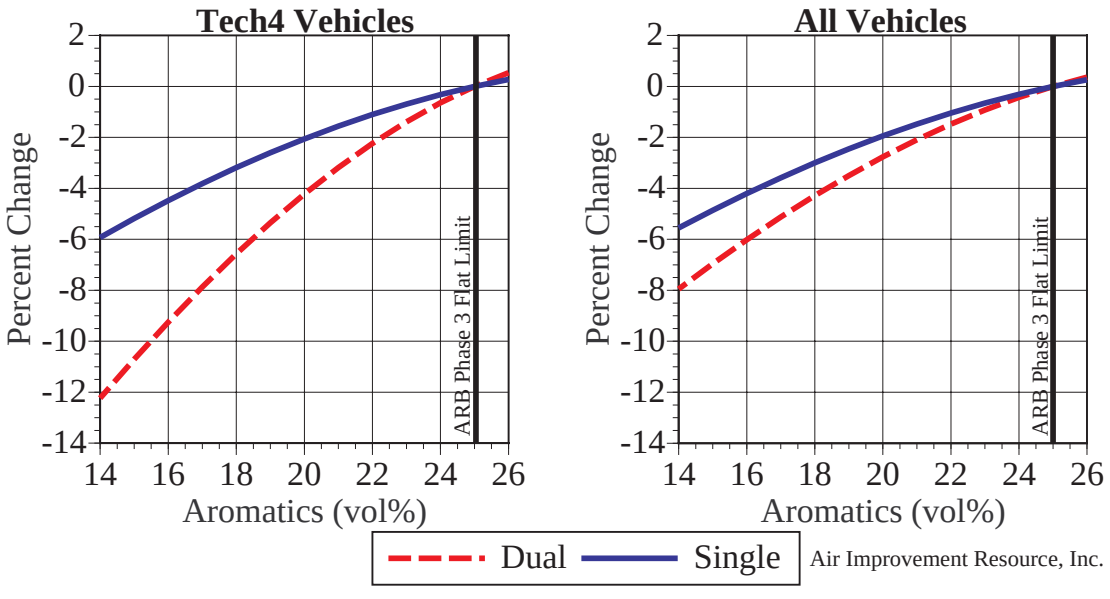
9.1 Comparison of Dual and Single Models for Fuel Properties where there are Significant Differences

In the following plots, we show a comparison of the dual model and the single model (ARB model). We do not show lower and higher emitting vehicles separately in the dual and single models, but only the weighted averages. Both models actually include lower and higher emitting vehicles; the difference is that the dual model breaks out their behavior separately, and then weights the behavior of the of lower and higher emitting vehicles with the weights that the EMFAC2007 model determines will be the situation in calendar year 2015, the evaluation year of the Predictive Model.

9.1.1 Aromatics - THC

The impact of the dual model on aromatics for both Tech 4 and for all vehicles is shown in the figure below. The dual model indicates a higher sensitivity to aromatics, i.e., as aromatics are reduced, THC is reduced more for the dual model than the single model. For all vehicles in 2015, the single model indicates that reducing aromatics from 25% to 20% reduces THC by 2%. The dual model reduces THC by 2.6%.

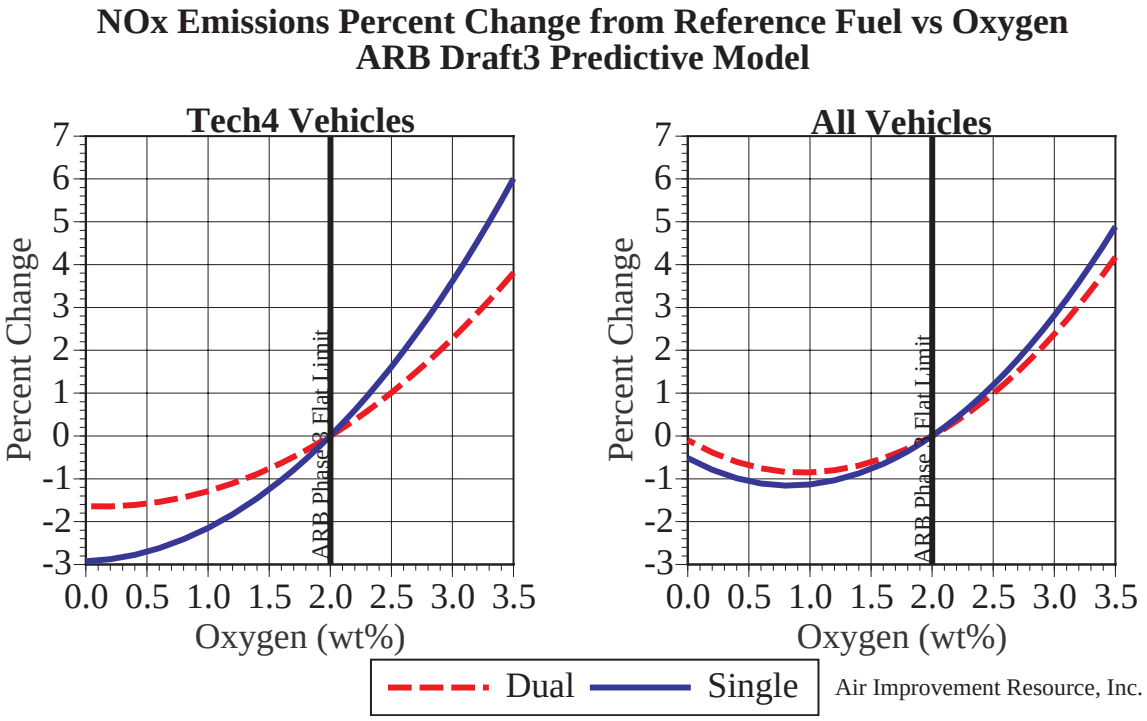
Exhaust THC Emissions Percent Change from Reference Fuel vs Aromatics
ARB Draft3 Predictive Model



This change in model sensitivity to aromatics is consistent with the literature and with the idea that aromatics change the equivalence ratio, making the exhaust stream richer, therefore, reductions in aromatics improve hydrocarbons on higher emitting vehicles more than normal emitting vehicles.

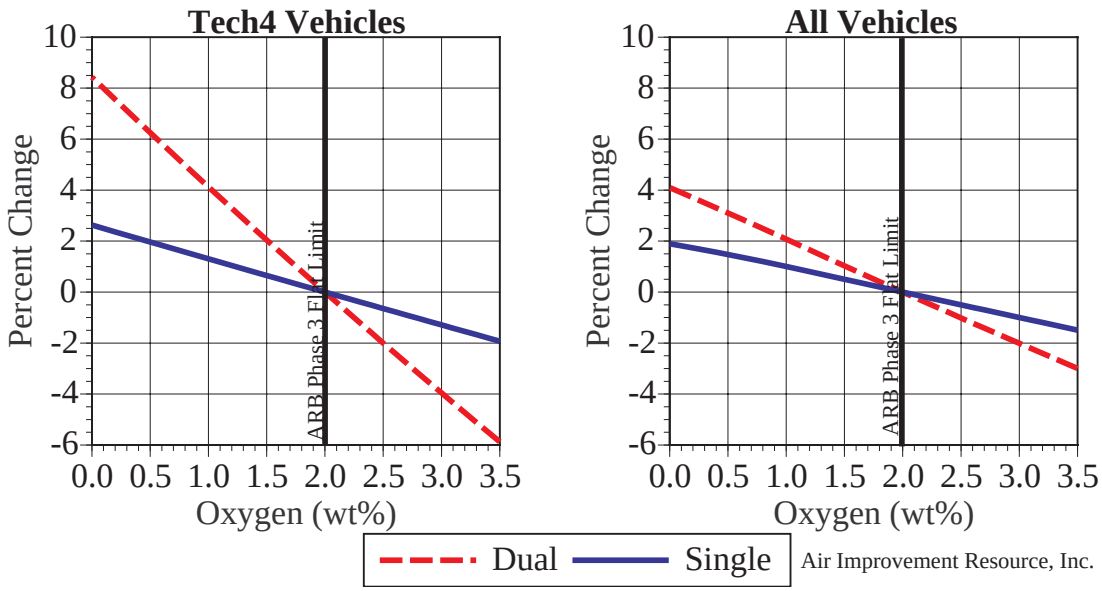
9.1.2 Ethanol - NOx and THC

The impact of the dual model on NOx and THC is shown in the two figures below. The dual model reduces the impact of oxygen on the NOx increase between and 2.0 percent and 3.5 percent. For Tech 5 vehicles, that impact is reduced from about 6% to less than 5%. This causes about a 0.5% reduction in the NOx increase for all vehicles in 2015.



The dual model also increases the THC reductions from increasing oxygen content between 2 percent and 3.5 percent. With the single model, THC is reduced by 2% when oxygen is increased from 2 percent to 3.5 percent. With the dual model, the reduction in THC for Tech 4 vehicles is nearly 5%. The extra oxygen is reducing unburned HC that is prevalent in higher HC emitting vehicles.

Exhaust THC Emissions Percent Change from Reference Fuel vs Oxygen
ARB Draft3 Predictive Model

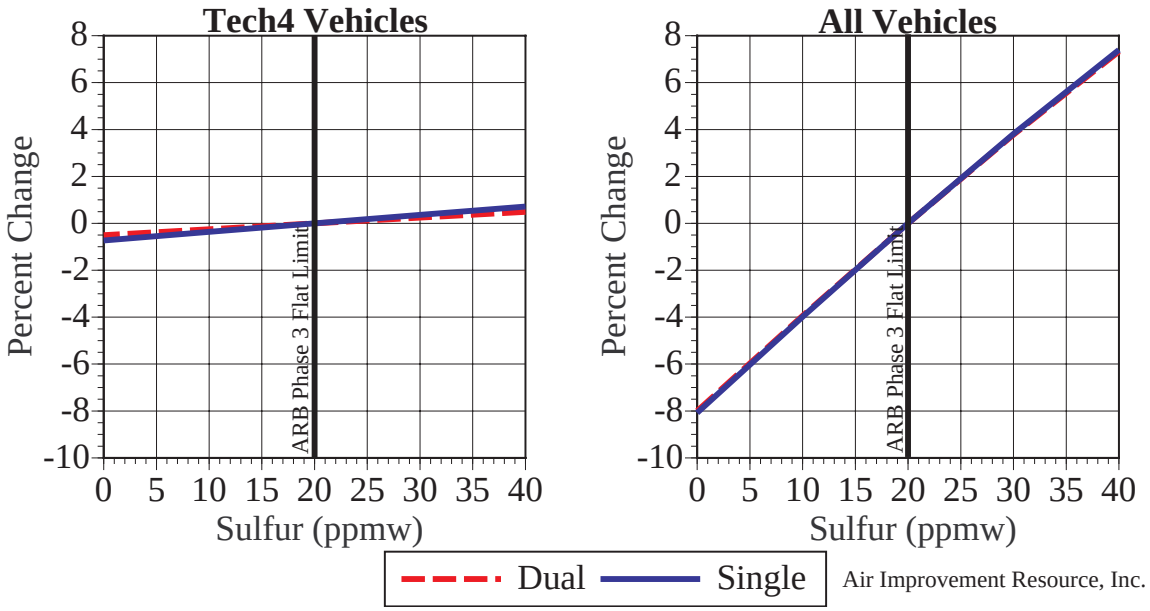


The changes in NOx and THC for oxygen are consistent with the idea that ethanol changes the equivalence ratio in the exhaust stream by making it leaner (opposite of aromatics). Thus, more oxygen is available to react the HC and CO in the exhaust. Also, since the catalytic converters of higher emitters are less functional than normal emitters, the exhaust stream enleanment due to the extra oxygen is less than it is on a normal emitting vehicle, leading to a lower NOx increase.

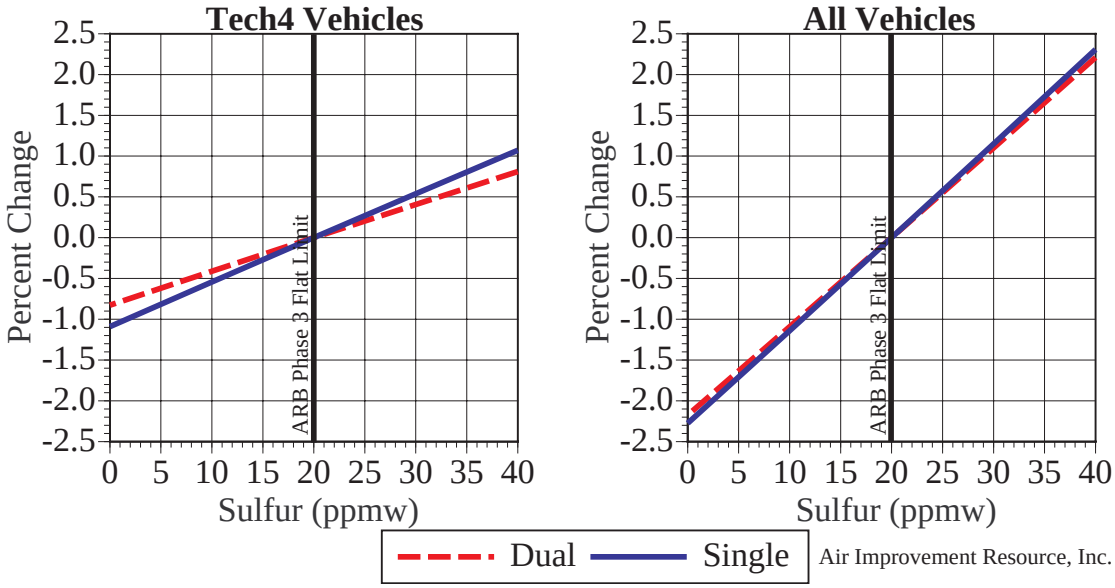
9.1.3 Sulfur - NOx and THC

The dual model reduces the impact of sulfur on THC and NOx from Tech 4 vehicles a small amount. This was expected, because sulfur reduces catalyst efficiency, and since higher emitting vehicles have lower catalyst efficiency, then sulfur affects their efficiency less than the higher efficiency catalysts of normal vehicles. As shown in the following two plots, however, the changes are quite small for sulfur.

NOx Emissions Percent Change from Reference Fuel vs Sulfur
ARB Draft3 Predictive Model



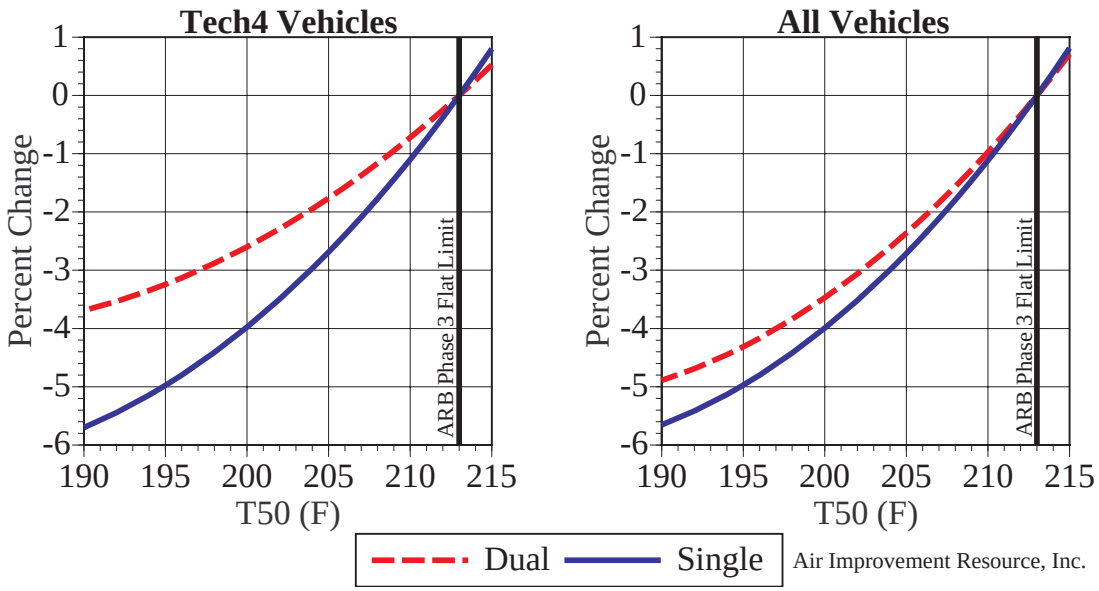
Exhaust THC Emissions Percent Change from Reference Fuel vs Sulfur
ARB Draft3 Predictive Model



9.1.4 T50 – THC Emissions

The dual model reduces the impact of reducing T50 on reducing THC emissions. A reduction in T50 from 213 to 205 reduces THC by 2.7% for Tech 4 vehicles for the single model, but about 2% for the dual model.

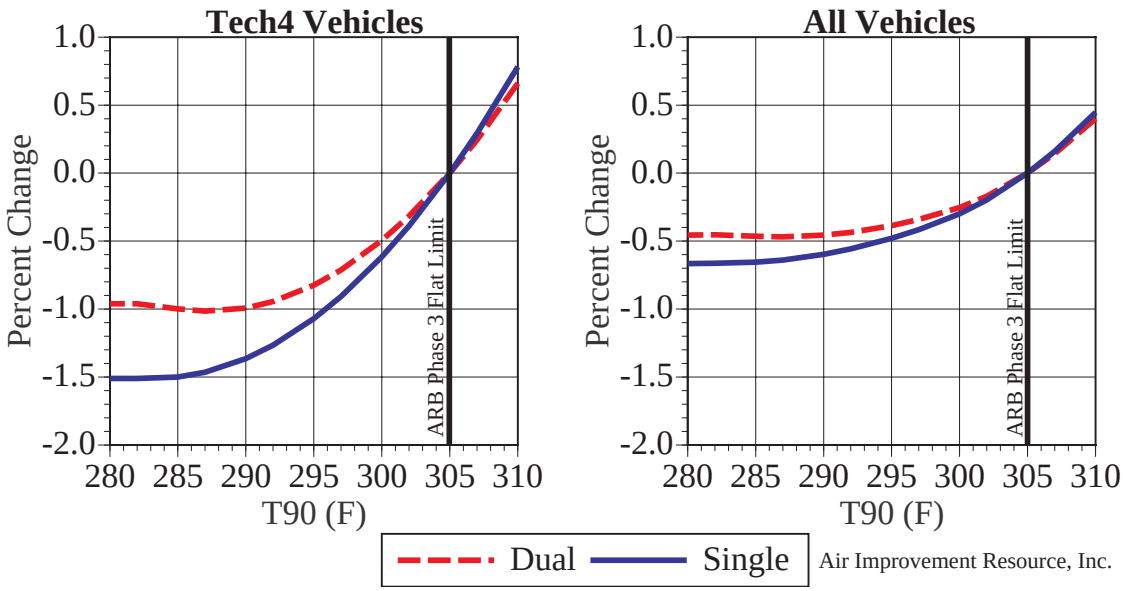
Exhaust THC Emissions Percent Change from Reference Fuel vs T50
ARB Draft3 Predictive Model



Since changes in distillation mainly affect emissions of either normal or higher emitting vehicles when they are warming up, it is not surprising that the impacts of T50 are less on a percentage basis for higher emitters than for normal emitters, since for higher emitters, the emissions during cold start and warm up are being divided by higher total emissions overall than for a normal emitter.

9.1.5 T90 – THC Emissions

The dual model also reduces the effect of lowering T90 on reducing THC emissions from tech 4 vehicles. This change is not very great between 295F and 305, but becomes greater at very low T90 levels.



The differences between normal emitting and higher emitting vehicles for T90 are consistent with the changes for T50, for the same reasons.

9.2 Comparison of 4 Example Passing Fuels Presented in Staff Report

The staff report shows four fuels from 0% ethanol to 10% ethanol that pass the single model, and the % reduction in ozone forming potential for these four fuels. We ran the properties of these four fuels through the dual model also. The results are presented in Table 12.

Table 12. Comparison of Single and Dual Model on Four Fuels passing the ARB Single Model				
	Percent Ethanol			
Property	0.0%	5.7%	7.7%	10.0%
RVP	6.60	6.91	6.92	6.99
T50	204	206	209	212
T90	315	310	313	313
Aromatic	25.0	25.0	25.0	25.0
Olefin	8.0	9.0	9.0	6.0
Total Oxygen	0.0	2.0	2.7	3.5
Sulfur	5	5	5	5
Benzene	0.50	0.50	0.50	0.50
Single Predictive Model Criteria	% Change in Emissions			
OFP	-0.67	-0.38	-0.59	-0.05
NOx	-6.0	-4.8	-2.9	-1.1
Pass/Fail	Pass	Pass	Pass	Pass
Dual Predictive Model Criteria	% Change in Emissions			
OFP	0.46	-0.25	-0.84	-0.71
NOx	-5.6	-4.8	-3.1	-1.5
Pass/Fail	Fail	Pass	Pass	Pass

We note that in these examples, ARB modified the distillation properties somewhat as the ethanol content changed. Aromatics were left unchanged at 25% (very near their current levels) but sulfur in these examples is 5 ppm, which is much lower than current sulfur, which is around 10-11 ppm.

The table shows that the 0.0% oxygen fuel does not pass the dual model criteria, while it does pass the single model criteria. The reason for this is that with the dual model, the T50 reductions employed in this example do not provide enough THC reductions. NOx reductions are also smaller (5.6% vs 6.0%) for the dual model, because Tech 4 higher emitters are being appropriately modeled as having less sensitivity to sulfur changes. There is no ethanol in this example, so there is no need to offset permeation. However, with a significant aromatics reduction from 25% to 19.6%, this fuel would pass the dual model.

For the 5.7% ethanol fuel, the OFP margin of 0.38% is cut slightly to 0.25%, and the NOx reduction is the same as the single model at 4.8%. The difference for OFP is again because T50 is not as effective with the dual model (i.e., higher Tech 4 emitters) as the single model for these examples, where aromatics are left unchanged. For the 7.7% and 10% examples, the dual model provides more margin for the OFP reduction than the single model, and indicates greater NOx reductions. Thus, for high levels of ethanol

(above 5.7% ethanol by volume), the dual model significantly improves the flexibility in meeting the Predictive Model criteria.

References

1. "Proposed 2007 Amendments to Phase 3 California Reformulated Gasoline Regulations, Staff Report: Initial Statement of Reasons, ARB, April 27, 2007.

2. "Fuel Effects in Auto/Oil High Emitting Vehicles", Knepper, Koehl, et.al, SAE930137.

3. "The Effect of Ethanol on a Spark Ignition Engine", Nakata, Ota, et.al., SAE2006-01-3380, October 16-19, 2006.

Attachment 1

MEMORANDUM

To: Statistics Working Group on California Air Resources Board Predictive Model

From: Jonathan Cohen

Date: 16 April, 2007

Re: Bootstrap p-value for difference in fuel effects between lower and higher NOx emitters in Tech 4.

I have submitted various updated calculations of the p-values for comparing the dual and single emissions models for Tech 4, most recently on March 19, 2007. To address concerns about the validity of the approximate likelihood ratio tests that I used, I present the results of 1,096 bootstrap simulations that demonstrate that the p-value for the test that the fuel responses are equal is less than one in 1,096.

Standard Analyses

In previous memoranda and presentations, I have presented the results of statistical tests comparing the fit of the ARB single model for Tech 4 (1986 to 1995 vehicles) with a dual model that fits separate models to lower emitters (where the NOx emissions on the fuel nearest to Auto/Oil fuel A are less than a given emissions cutoff, and higher emitters (other vehicles).

To test whether the higher emitters have different intercepts or fuel coefficients than lower emitters, a standard test statistic is

VF = twice the log-likelihood for the dual model minus twice the log-likelihood for the single model.

The p-value for VF can be approximated by comparing VF to a chi-square distribution with d degrees of freedom, where d is the additional number of parameters (for the fixed and random effects). It is not clear whether d should include all fitted parameters or should exclude any of the covariance parameters that are estimated to be zero. In either case, p-values well below
10^{-10} were found for all the cutoffs evaluated. This result should not be unexpected since by definition the higher emitters have a higher average for the nearest fuel to fuel A, which usually implies a higher average intercept, even if the fuel coefficients are different. The calculated p-value for this analysis is clearly overstated, since it does not take into account the fact that the higher emitters were deliberately selected to have different (higher) vehicle intercepts. (Although higher emitters have been defined on the basis of their emissions on the nearest fuel to fuel A, for most vehicles this is effectively

the same as using the vehicle intercept, because vehicle-to-vehicle variability is much larger than fuel-to-fuel variability on the same vehicle.) In fact, the bootstrap analyses described below showed that the true p-values for different intercepts or fuel coefficients were about 0.5 or higher.

To test whether the higher emitters have different fuel coefficients than lower emitters, i.e., different fuel responses, a standard test statistic is

F = twice the log-likelihood for the dual model minus twice the log-likelihood for the single model with different intercepts.

The single model with different intercepts is defined by fitting the ARB model with extra fixed and random effects for the higher and lower vehicle intercepts. Lower emitters are assumed to have vehicle intercepts drawn randomly from a normal distribution with mean m1 and variance v1. Higher emitters are assumed to have vehicle intercepts drawn randomly from a normal distribution with mean m2 and variance v2. I used the following SAS code to fit the single model with different intercepts:

```
PROC MIXED MAXITER=500 METHOD=ml NOCLPRINT ;
CLASS NEW lower;
MODEL LN_NOx = lower RV T5 T9 AR OL OX SU t5t5 t9ar suox arsu oxox susu
        /S DDFM=RES;
RANDOM
RV T5 T9 AR OL OX SU t5t5 t9ar suox arsu oxox susu
/SUB=NEW;
random int / group=lower sub=new;
run;
```

where "lower" equals 1 for lower emitters and equals 0 for higher emitters. "New" is the unique study/vehicle identifier, defined by concatenating study and vehicle.

The dual model differs from the single model with different intercepts by allowing the fuel coefficients to be different for lower and higher emitters. Thus the statistic F provides a test of whether lower and higher emitters respond the same to fuel changes.

The p-value for F can be approximated by comparing F to a chi-square distribution with d degrees of freedom, where d is the additional number of parameters (for the fixed and random effects). It is not clear whether d should include all fitted parameters or should exclude any of the covariance parameters that are estimated to be zero. In either case, p-values well below
10^{-15} were found for all three pollutants at the optimal cutoffs (that produced the dual model with the highest log-likelihood). This shows that higher emitters respond differently to fuel changes than lower emitters.

Concerns have been raised by David Rocke (personal communication) that the p-values may not be accurately estimated by these procedures. Some reasons why these calculations may be inaccurate are:

- The chi-square distribution for the likelihood ratio test is an approximation for large samples.

- The asymptotics may not apply in cases where the estimated parameter values are on the boundary of the parameter space (in this case, some of the estimated covariance parameters are zero).

- The emissions data are used twice, to subdivide vehicles into lower and higher emitters and again to fit the separate lower and higher emitter models.

- The selection of the optimal cut-off based on finding the fitted dual model with the highest log-likelihood may impact the distribution of the statistics VF and F.

To address these concerns, the following bootstrap procedure, suggested by David Rocke, was applied.

Bootstrap

This bootstrap procedure was applied to evaluate the p-value for the fuel effect difference summary statistic F and the NOx dual model. The optimal dual model (highest log-likelihood) had a cutoff of 0.6 g/mi, 60 % of the 1 g/mile standard.

Two approaches were evaluated. In the first approach, we followed the same procedure as the original dual model approach, defining the vehicle's emissions level by the simulated observed NOx emissions on the nearest fuel to fuel A, defined by the Euclidean distance between the seven fuel parameters on each tested fuel and Auto/Oil fuel A. In the second approach, we used the simulated vehicle intercepts and fuel effects to estimate the expected value on Auto/Oil fuel A for that vehicle, i.e., the average of infinitely many tests on fuel A. For the simulated data, this expected value is easily estimated for each vehicle, even though the actual vehicle may not have been tested on that fuel. In the second approach, the vehicle's emission level is defined by the expected emissions on fuel A.

For each simulation, the following procedure was applied:

1. Simulate data from the ARB model.

2. Fit the ARB single model to the simulated data (using maximum likelihood).

3. For each vehicle, use the simulated emissions on the nearest fuel to fuel A to determine the vehicle's emissions level.

4. For each of the following cutoffs, fit the dual model (i.e., the single model separately fitted to lower and higher emitters), and the single model with different intercepts: 30%, 40%, … 120% of the NOx standard 1 g/mile. Use maximum likelihood, not restricted maximum likelihood, in all cases.

5. Compute the log-likelihood for the dual models, by summing the log-likelihoods for the fitted lower and higher emitter models. Find the optimal cutoff as the dual model with the highest log-likelihood.

6. Compute the statistic F, twice the log-likelihood for the dual model minus twice the log-likelihood for the single model with different intercepts.

7. For each vehicle, use exp of the expected emissions on fuel A to determine the vehicle's NOx emissions level.

8. For each of the following cutoffs, fit the dual model (i.e., the single model separately fitted to lower and higher emitters), and the single model with different intercepts: 30%, 40%, … 120% of the NOx standard 1 g/mile. Use maximum likelihood, not restricted maximum likelihood, in all cases.

9. Compute the log-likelihood for the dual models, by summing the log-likelihoods for the fitted lower and higher emitter models. Find the optimal cutoff as the dual model with the highest log-likelihood.

10. Compute the statistic F, twice the log-likelihood for the dual model minus twice the log-likelihood for the single model with different intercepts.

To simulate the emissions data, we proceeded as follows: The ARB single model has 14 fixed and 14 random fuel terms, including the intercepts. The Tech 4 data base has 900 vehicles, or, more precisely, 900 vehicle/study combinations. For each vehicle, and each fuel term, the fuel coefficient or intercept for that vehicle is independently drawn from a normal distribution where the mean is the estimated fixed effect parameter and the variance is the estimated random effect parameter (covariance parameter). For each of the 4,185 vehicle and fuel combinations, the mean log (NOx) is calculated as simulated vehicles' intercept plus the sum of the normalized fuel term times the simulated vehicle's fuel coefficient. The log(NOx) is simulated by adding a normally distributed residual error term with mean zero and variance V, the residual error covariance parameter.

Although the original dual models were fitted with cutoffs ranging from 20% to 200%, the twice likelihoods were 2,980 to 3,345 for the selected cutoffs (30%, 40%, … 120%) and at most 2,960 for the other cutoffs, so it was felt that simulating additional cutoffs would be an unnecessary cost in execution time. Since the simulated optimal dual model cutoff ranged from 40% to 70%, this assumption is justified.

The complete procedure was applied to 1,100 simulations. However, 4 simulations were rejected because the maximum likelihood procedure failed to converge for at least one of the fitted models.

Results

The statistic F for the original optimal dual model was equal to 206.07. Using the simulated observed emissions on the nearest fuel to fuel A to define the emissions levels, the 1,096 simulations of F had values ranging from 10.00 to 58.40. The optimal cutoff for that approach ranged from 40% to 60%. Using the expected emissions on fuel A to define the emissions levels, the 1,096 simulations of F had values ranging from 8.29 to 61.60. The optimal cutoff for that approach ranged from 50% to 70%. In either case the bootstrap p-value for the test of equal fuel effects is less than 1/1096. The p-value can be expected to be much lower than 1/1096, since the highest simulated value of F was only 61.60, which is much lower than the test value of 206.07.

Attachment 2

MEMORANDUM

To: California Air Resources Board

From: Jonathan Cohen

Date: 21 March, 2007

Re: Tech 4 Dual Models for Delta NOx. Revision 2.

This memorandum addresses one of the concerns that has been expressed about the dual model approach, namely that the estimated coefficients are potentially biased since the "independent" variables and the error terms are not independent. An alternative modeling approach, based on predicting differences in log(NOx) between pairs of fuels on the same vehicle, is presented that eliminates this problem and gives very similar predictions to the original dual model approach.

This version is a revision of the previous memorandum, dated 9 March, 2007. In the previous version, the error terms in the Delta model were assumed to be independent. In this revised version, the Delta model error structure follows directly from the error structure of the original dual model and the predicted effects match the original dual model even more closely.

Statistical Issue

The dual model approach for Tech 4 has been presented several times to the Air Resources Board, most recently in my fuels workshop presentation "Uncertainties of Oxygen-NOx Effect from Predictive Model", presented 22 September, 2006, and the accompanying document "Uncertainties of Oxygen-NOx effect from Predictive Model studies," dated 18 September, 2006. The basic idea is to fit separate mixed models to Tech 4 higher and normal emitters, defined as vehicles emitting NOx greater than or less than a selected cut-off value. The original cut-off value of 1 g/mile was selected for compatibility with the EMFAC model emitter groups. Various other cut-off values have been considered, ranging from 0.4 to 2 g/mile, but all of them consistently exhibit an extremely statistically significant improved fit compared to the ARB single model approach and show a lower response to oxygen for the higher emitter vehicles.

One statistical issue that has been raised is the possibility of biased inferences caused by correlations between the "independent" variables and the error terms, since the same data are used to define the higher/normal emitter groups and then to fit the two models. In a Predictive Model Statistics Working Group conference call, Professor Rocke from the University of Davis mentioned this issue but said this may not be a problem since differences between vehicles have much more of an effect on emissions than differences between fuels on the same vehicle. However, in an later email he wrote:

"It is well known that introducing functions of the response on the RHS of a regression can cause inferences that are incorrect, including apparent "statistical significance" that does not reflect the true stochastic properties of the model. While there are reasons to argue that this may possibly not occur here, it seems to me that the burden of proof is on the proposer of this to show it is not a problem in this case."

In this memorandum we present an alternative modeling approach that indeed shows that this statistical inference issue is not a problem in this case.

Dual and Delta Models

The latest version of the ARB draft Tech 4 NOx model has all seven main effects plus the following six interaction terms: OXOX, SUOX, T5T5, SUSU, T9AR, ARSU. For example, OXOX is the square of the (normalized) oxygen term and SUOX represents SU times OX, i.e., the variation of the oxygen effect with different levels of sulfur. The fuel parameters were renormalized to a mean of zero and a variance of 1. The model takes the general mixed form:

$$\text{Log(NOx) (vehicle V, fuel F)} = \text{int(V)} + \Sigma\, \beta_i(V)\, EFF_i(F) + \text{Error(V, F)} \quad (1)$$

where $EFF_i(F)$ denotes the i'th fuel effect term for fuel F, and where int(V) and $\beta_i(V)$ are the vehicle-specific intercepts and slopes that are assumed to each have a normal distribution across the entire California fleet. The errors are assumed to have a normal distribution with mean zero across all vehicle and fuel tests. For the condensed data used in the latest version of the predictive model, the NOx data values are averages across each vehicle and fuel combination. The predictive model only uses the fuel parameter fixed effects, i.e., the fleet means of the $\beta_i(V)$. Equation 1 describes the "Original Single" model.

For a given vehicle, let fuel A* denote the closest fuel to fuel A as defined in Jonathan Cohen's memorandum "Uncertainties of Oxygen-NOx effect from Predictive Model studies," dated 18 September, 2006. The Dual model fits equation 1 separately for higher and normal emitters defined by whether or not NOx (vehicle V, fuel A*) $\geq$ C, the cut-off. For the analyses presented in this memorandum C = 1 g/mile.

The Delta version of the dual model is obtained by taking fuel differences, as follows. From Equation 1,

$$\text{Log(NOx) (vehicle V, fuel F)} - \text{Log(NOx) (vehicle V, fuel A*)} = \Sigma\, \beta_i(V)\, \{EFF_i(F) - EFF_i(A^*)\} + \text{Error(V, F)} - \text{Error(V, A*)}. \quad (2)$$

The slopes $\beta_i(V)$ are the vehicle-specific slopes that are assumed to have a normal distribution across the entire California fleet. The terms Error(V, F) are residual error

terms that have a normal distribution across all vehicle and fuel tests with mean zero and variance VERR, say. The terms −Error(V, A*) can be regarded as random intercept terms that have a normal distribution across the entire California fleet with mean zero and variance VERR. This model for the log(NOx) fuel differences has exactly the same structure as Equation 1, except for two restrictions: the mean vehicle intercept is zero (i.e., the fixed effects model has no intercept) and the residual variance equals the variance of the vehicle intercepts. This model, including both the restrictions, was fitted using SAS 9.1.

The Delta Single model fits the mixed model in Equation 2 to all the Tech 4 data except for the tests on fuel A* on each vehicle, where Delta = 0 by definition. The Delta Dual model fits the mixed model in Equation 2 separately to the higher and normal emitters, again excluding the tests on fuel A* on each vehicle. Assume that the differences Log(NOx) (vehicle V, fuel F) − Log(NOx) (vehicle V, fuel A*) are statistically independent of the fuel A* values Log(NOx) (vehicle V, fuel A*). Then the responses in Equation 2 are independent of the higher and normal emitter indicators, *so the bias issue does not apply to this model*.

Equation 2 can easily be used to make fleet average fuel effect predictions for use in the Predictive Model. Let C denote the base fuel. Let B_i denote the i'th fixed effect, i.e., the fleet average of $\beta i(V)$. Then the fleet average for fuel F minus the fleet average for the base fuel is estimated by

$$
\begin{aligned}
&E\{\text{ Log(NOx) (vehicle V, fuel F) } - \text{Log(NOx) (vehicle V, fuel C)}\} = \\
&E\{\text{ Log(NOx) (vehicle V, fuel F) } - \text{Log(NOx) (vehicle V, fuel A*)}\} - \\
&E\{\text{ Log(NOx) (vehicle V, fuel C) } - \text{Log(NOx) (vehicle V, fuel A*)}\} \\
&= \Sigma\, B_i\, \{EFF_i(F) - EFF_i(A^*)\} - \Sigma\, B_i\, \{EFF_i(C) - EFF_i(A^*)\} \\
&= \Sigma\, B_i\, \{EFF_i(F) - EFF_i(C)\}.
\end{aligned}
$$

For the Dual model calculations presented here, the same set of fuel effects terms were fitted in all the models (although the Delta models replaced each fuel effect term by the difference between the same term calculated on fuels F and A*). This approach allows the coefficients to be directly compared. In a final application of these ideas for the Predictive Model, it would be reasonable to apply the usual stepwise approach to each model to make the models parsimonious and exclude non-significant fixed effect quadratic or interaction terms.

Results

The fixed effects coefficients for the single, higher, and normal emitter models using the original Dual model and the new Delta Dual model are presented in the Appendix. It can be seen that the corresponding coefficients for the original and Delta models match well except for very non-significant terms such as the T5, T9, and RV main effects. Note that these models have a different set of model terms than those used in the document "Uncertainties of Oxygen-NOx effect from Predictive Model studies," dated 18

September, 2006, due to ARB's more recent revisions of the model formulation (to exclude OLOL terms from the stepwise model development).

The oxygen-NOx effects can be calculated from these model coefficients. The following table gives the estimated percentage change in NOx as the oxygen weight percent increases from 2 to 3.5 %, all other fuel parameters being held fixed. Estimates are provided for the original and Delta models using a single model for all vehicles and also using separate models for the normal and higher emitter vehicles. Estimates are also provided for the Dual model, combining the normal and higher emitters assuming that 20.7 % of emissions are from normal emitters and 79.3 % of emissions are from higher emitters. These emission contribution calculations (from Graboski, Cohen and Pollack, 2000[5]) use the earlier EMFAC 2000 version of the EMFAC model and are based on the year 2005. In the EMFAC 2000 models, the combined Moderate, High, Very High, and Super NOx emitter categories contain all vehicles emitting more than 1 g/mile NOx, i.e., the higher emitter vehicles as defined in this memorandum.

Model	**Emitters**	**% Change in NOx**
Original Single	All	6.01 %
Original Dual	Normal	6.77 %
Original Dual	Higher	0.25 %
Original Dual	All	1.60 %
Delta Single	All	6.04 %
Delta Dual	Normal	6.64 %
Delta Dual	Higher	0.27 %
Delta Dual	All	1.58 %

Using the Delta Dual model, the estimated oxygen-NOx effects are very close to those using the original Dual model.

[5] Graboski M. S., J. Cohen, and A. Pollack. June 2000. *The Effect of Removing Oxygen from California RFG3 on Light-Duty Mobile Source NOx, VOC, and Ozone Emissions: The Impact of High Emitting Vehicles.*

APPENDIX: FIXED EFFECT COEFFICIENTS

Original Single

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.6338	0.02299	4171	-27.57	<.0001
OX	0.01454	0.003065	4171	4.75	<.0001
OXOX	0.01072	0.003760	4171	2.85	0.0044
AR	0.01766	0.004868	4171	3.63	0.0003
SU	0.04671	0.004592	4171	10.17	<.0001
OL	0.01718	0.002465	4171	6.97	<.0001
T5	-0.00243	0.003781	4171	-0.64	0.5206
T9	0.002083	0.003569	4171	0.58	0.5596
RV	0.004547	0.004065	4171	1.12	0.2634
SUOX	-0.01346	0.002914	4171	-4.62	<.0001
T5T5	0.006274	0.001792	4171	3.50	0.0005
SUSU	-0.00499	0.001813	4171	-2.75	0.0059
T9AR	-0.00289	0.001324	4171	-2.18	0.0291
ARSU	0.005974	0.002961	4171	2.02	0.0437

Delta Single

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
OX	0.01434	0.003075	3272	4.67	<.0001
OXOX	0.01057	0.003788	3272	2.79	0.0053
AR	0.01838	0.004888	3272	3.76	0.0002
SU	0.04812	0.004657	3272	10.33	<.0001
OL	0.01732	0.002468	3272	7.02	<.0001
T5	-0.00284	0.003760	3272	-0.75	0.4508
T9	0.002075	0.003578	3272	0.58	0.5620

	RV	0.002400	0.004048	3272	0.59
0.5533					
	SUOX	-0.01417	0.002925	3272	-4.85
<.0001					
	T5T5	0.006445	0.001787	3272	3.61
0.0003					
	SUSU	-0.00529	0.001819	3272	-2.91
0.0037					
	T9AR	-0.00284	0.001324	3272	-2.14
0.0322					
	ARSU	0.006177	0.002965	3272	2.08
0.0373					

Orig Dual Normal

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	-0.8002	0.02075	3518	-38.56	<.0001
OX	0.01687	0.003305	3518	5.10	<.0001
OXOX	0.01399	0.004194	3518	3.33	0.0009
AR	0.01410	0.005177	3518	2.72	0.0065
SU	0.04947	0.005632	3518	8.78	<.0001
OL	0.02050	0.003097	3518	6.62	<.0001
T5	-0.00215	0.004041	3518	-0.53	0.5946
T9	0.002193	0.004098	3518	0.54	0.5926
RV	0.008526	0.004859	3518	1.75	0.0794
SUOX	-0.01072	0.003220	3518	-3.33	0.0009
T5T5	0.006284	0.001896	3518	3.31	0.0009
SUSU	-0.00441	0.002610	3518	-1.69	0.0910
T9AR	-0.00314	0.001442	3518	-2.18	0.0293
ARSU	0.007389	0.003330	3518	2.22	0.0266

Delta Dual Normal

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|

OX	0.01631	0.003312	2741	4.92	<.0001
OXOX	0.01306	0.004207	2741	3.10	0.0019
AR	0.01574	0.005188	2741	3.03	0.0024
SU	0.05436	0.005756	2741	9.44	<.0001
OL	0.02070	0.003077	2741	6.73	<.0001
T5	-0.00399	0.004006	2741	-1.00	0.3195
T9	0.003234	0.004113	2741	0.79	0.4317
RV	0.001343	0.004851	2741	0.28	0.7819
SUOX	-0.01207	0.003232	2741	-3.73	0.0002
T5T5	0.006450	0.001885	2741	3.42	0.0006
SUSU	-0.00589	0.002626	2741	-2.24	0.0249
T9AR	-0.00306	0.001441	2741	-2.12	0.0340
ARSU	0.007787	0.003335	2741	2.34	0.0196

Attachment 3
Weighting Factor Calculations

California, 2015 Summer, LDA+LDT1+LDT2

Emission Level	Data	MY Group			
		1985-	1986-1995	1996+	All
All Emitters	Population	453,324	2,139,115	21,361,524	23,953,962
	VMT (Miles/Day)	8,569,354	48,877,838	766,898,653	824,345,845
	Exhaust TOG (Tons/Day)	22.1	38.8	54.6	115.5
	Evap TOG (Tons/ay)	22.6	72.9	81.2	176.7
	Total TOG (Tons/Day)	44.7	111.8	135.8	292.3
	CO (Tons/Day)	344.1	629.2	1,423.1	2,396.4
	NOx (Tons/Day)	22.0	65.5	115.8	203.4
0.6 * Standard	Exhaust TOG (Tons/Day)	12.3	11.2	24.6	48.2
	Evap TOG (Tons/ay)	5.6	4.8	20.2	30.6
	Total TOG (Tons/Day)	17.9	16.0	44.8	78.8
	CO (Tons/Day)	151.3	428.2	1,015.6	1,595.1
	NOx (Tons/Day)	14.0	31.4	32.0	77.4
1.0 * Standard	Exhaust TOG (Tons/Day)	13.1	16.4	32.0	61.5
	Evap TOG (Tons/ay)	7.7	18.7	25.2	51.7
	Total TOG (Tons/Day)	20.8	35.2	57.3	113.2
	CO (Tons/Day)	180.1	457.9	1,097.4	1,735.4
	NOx (Tons/Day)	15.1	38.9	53.0	107.1
1.6 * Standard	Exhaust TOG (Tons/Day)	14.1	24.2	43.1	81.4
	Evap TOG (Tons/ay)	10.9	39.6	32.8	83.3
	Total TOG (Tons/Day)	25.0	63.8	75.9	164.7
	CO (Tons/Day)	223.4	502.3	1,219.9	1,945.7
	NOx (Tons/Day)	16.8	50.2	84.5	151.6
2.0 * Standard	Exhaust TOG (Tons/Day)	14.8	29.4	50.4	94.7
	Evap TOG (Tons/ay)	13.0	53.6	37.8	104.4
	Total TOG (Tons/Day)	27.8	83.0	88.3	199.1
	CO (Tons/Day)	252.3	532.0	1,301.7	2,086.0
	NOx (Tons/Day)	17.9	57.8	105.6	181.3
All Non-Normals	Exhaust TOG (Tons/Day)	22.8	43.0	66.1	131.8
	Evap TOG (Tons/ay)	48.8	115.1	2,585.5	2,749.4
	Total TOG (Tons/Day)	71.6	158.0	2,651.6	2,881.2
	CO (Tons/Day)	423.5	975.7	2,405.8	3,805.0
	NOx (Tons/Day)	28.9	80.8	186.5	296.2

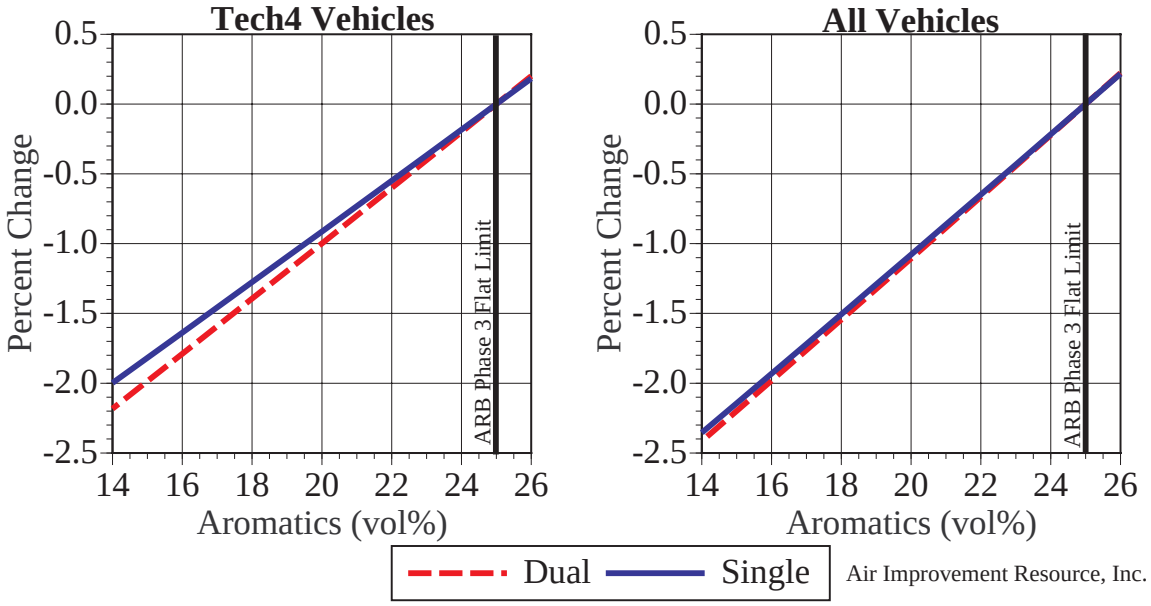
California, 2015 Summer, LDA+LDT1+LDT2

Standard Factor	Data	"A" Coefficient MY Group			
		1985-	1986-1995	1996+	All
1.0	Exhaust TOG	0.072	0.155	0.337	0.232
1.0	Evap TOG	0.636	0.438	0.978	0.954
1.0	Total TOG	0.528	0.377	0.970	0.935
1.6	CO	0.397	0.732	0.829	0.758
0.6	NOx	0.461	0.309	0.458	0.424

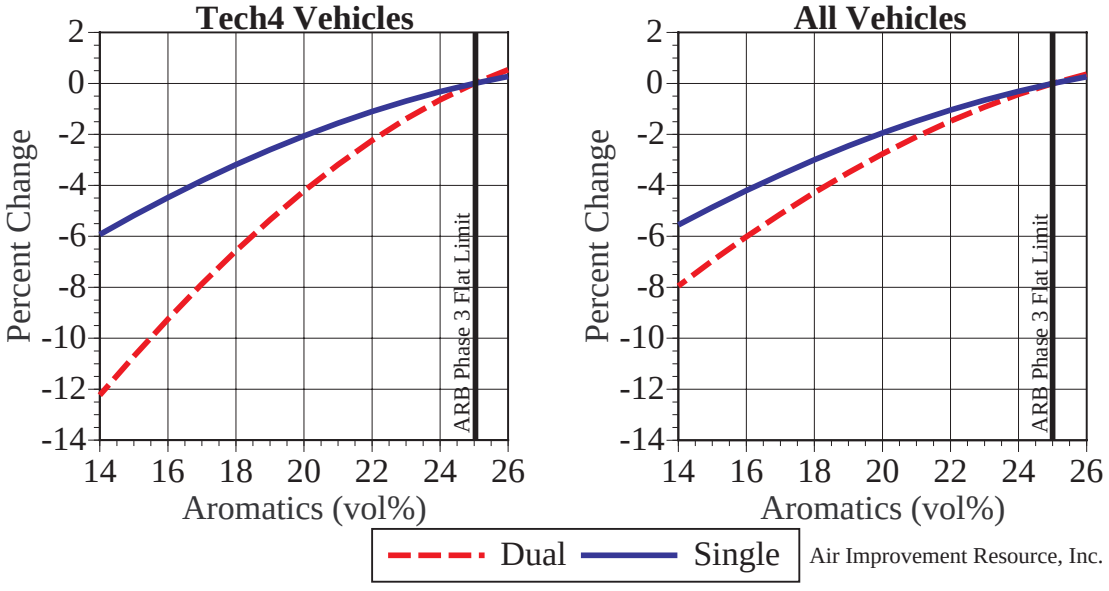
Attachment 4
Comparison of Single and Dual Model

The following plots compare the ARB single model and the dual model. The plots aare presented in pairs, where the plot on the left is for Tech 4 vehicles only, and the plot on the right is for all vehicles in 2015.

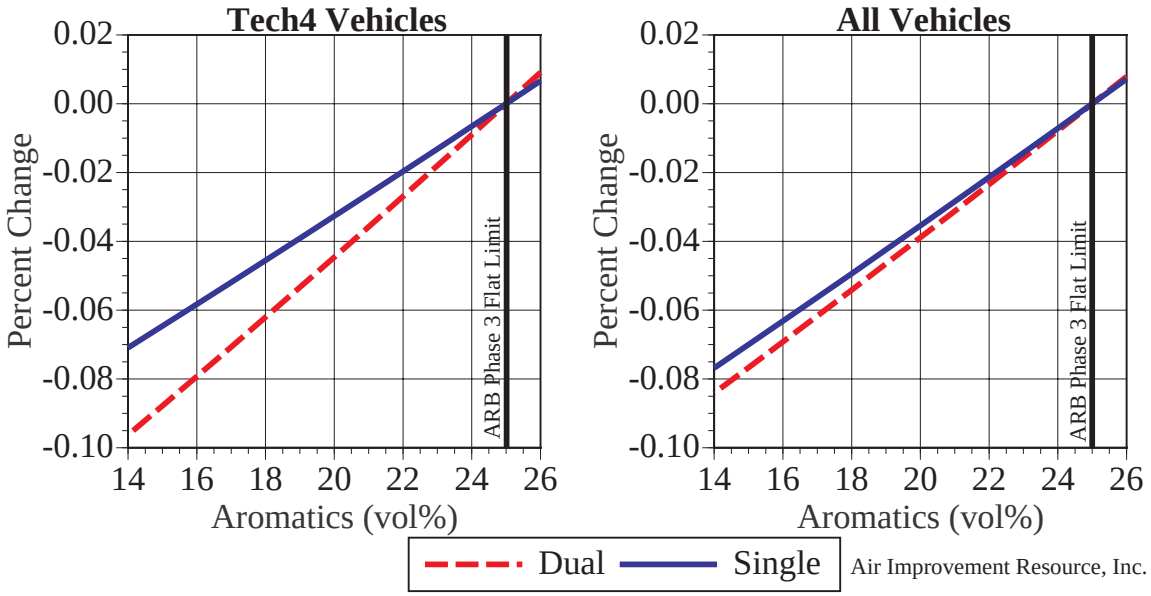
NOx Emissions Percent Change from Reference Fuel vs Aromatics
ARB Draft3 Predictive Model



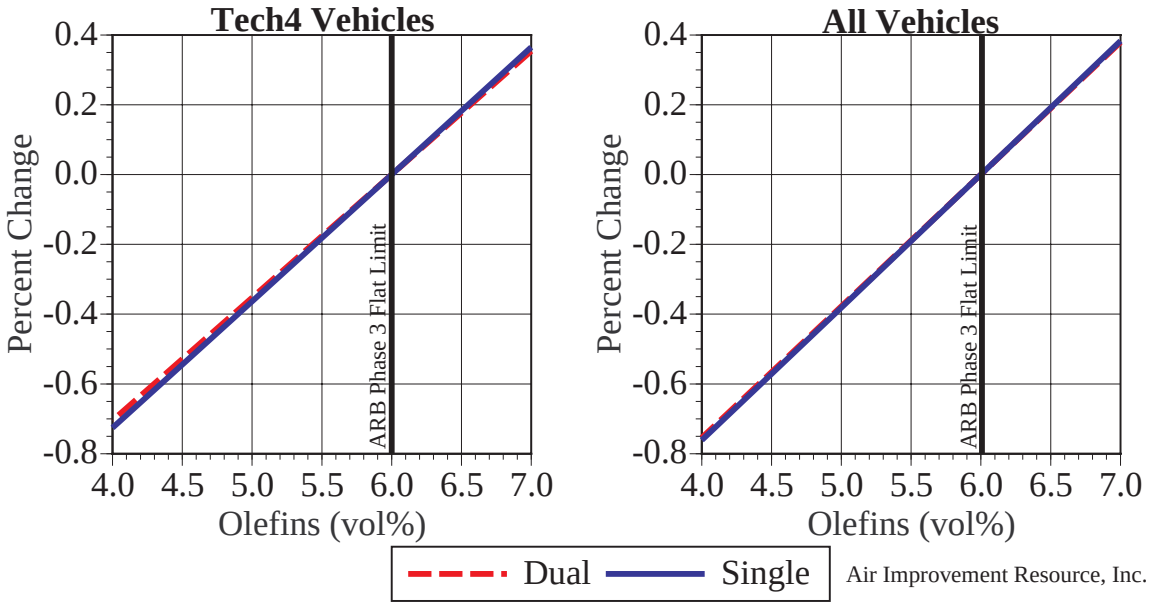
Exhaust THC Emissions Percent Change from Reference Fuel vs Aromatics
ARB Draft3 Predictive Model



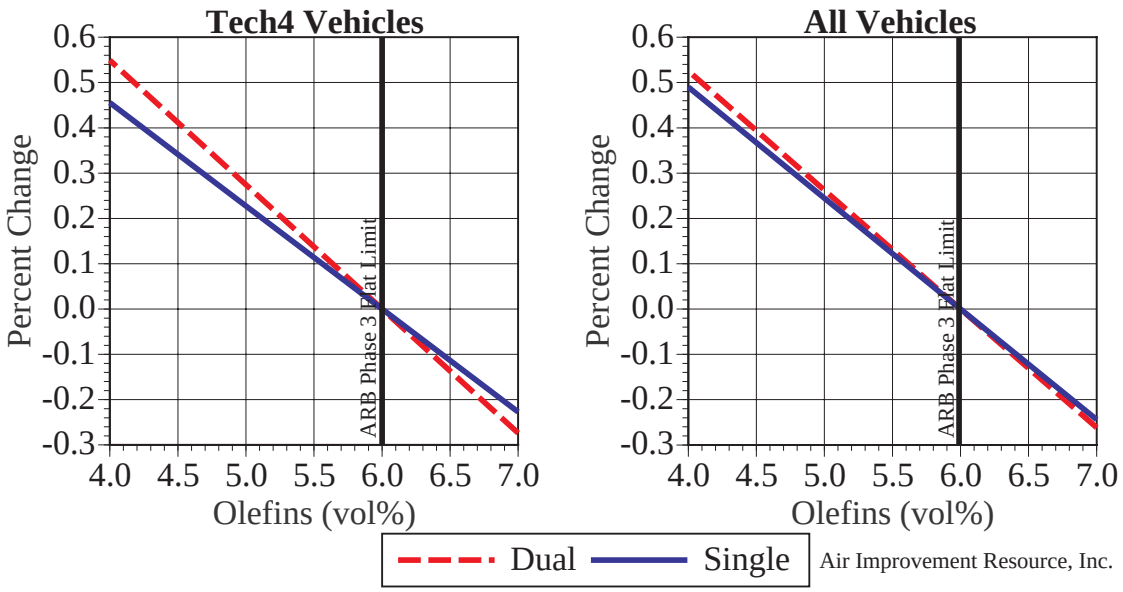
CO Emissions Percent Change from Reference Fuel vs Aromatics
ARB Draft3 Predictive Model



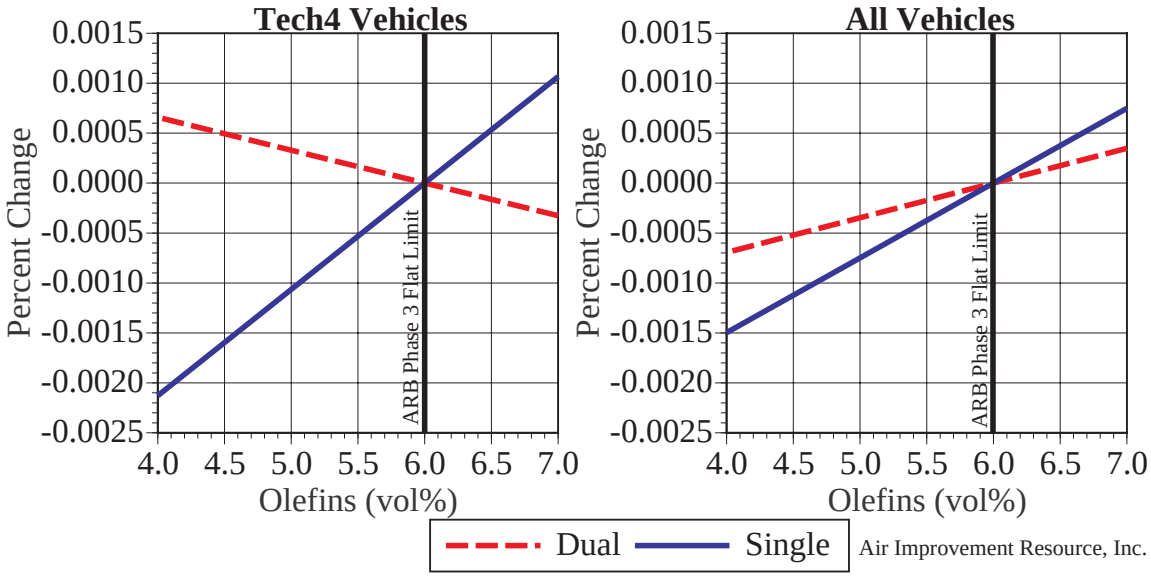
NOx Emissions Percent Change from Reference Fuel vs Olefins
ARB Draft3 Predictive Model



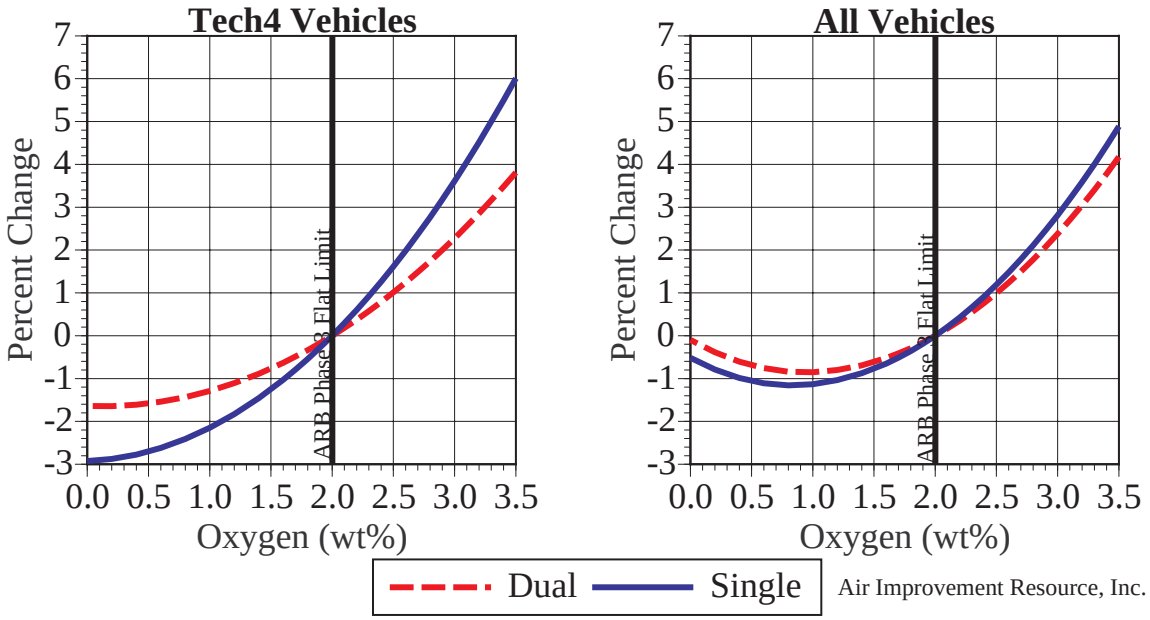
Exhaust THC Emissions Percent Change from Reference Fuel vs Olefins
ARB Draft3 Predictive Model



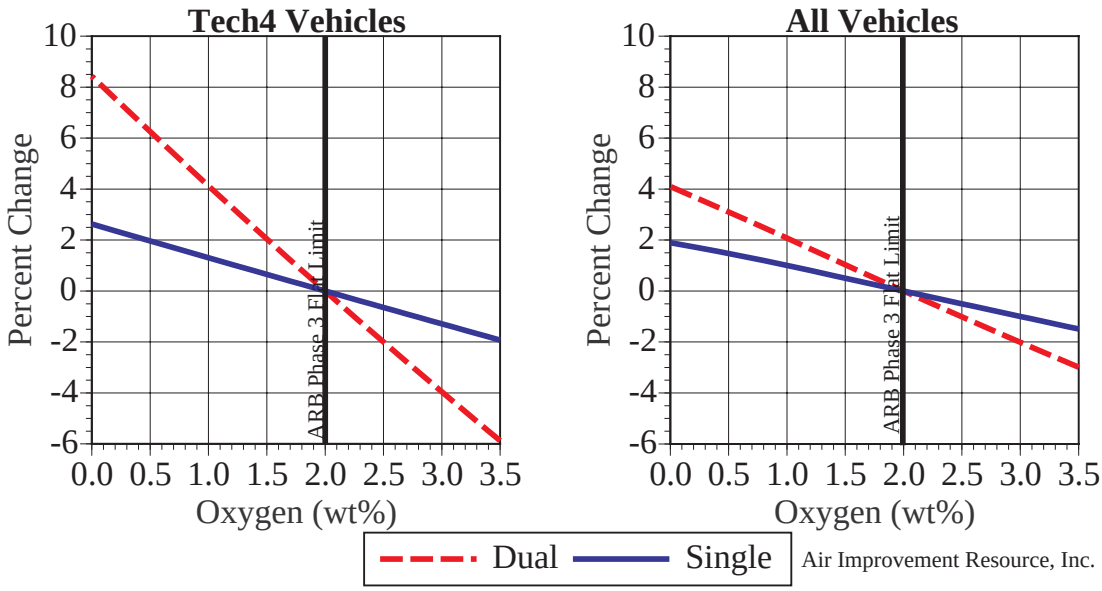
CO Emissions Percent Change from Reference Fuel vs Olefins
ARB Draft3 Predictive Model



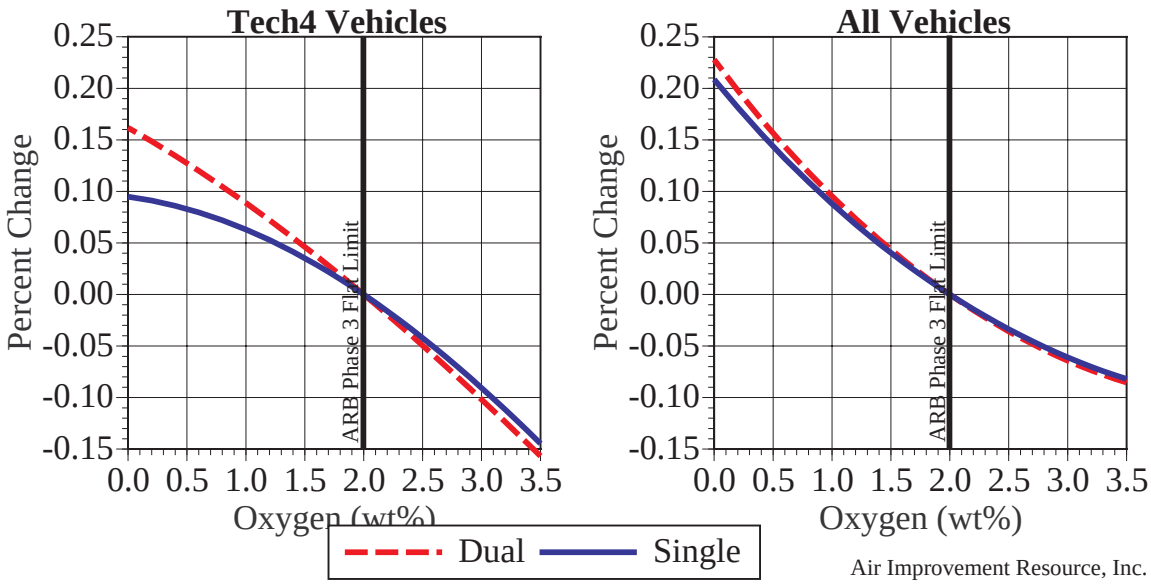
NOx Emissions Percent Change from Reference Fuel vs Oxygen
ARB Draft3 Predictive Model



Exhaust THC Emissions Percent Change from Reference Fuel vs Oxygen
ARB Draft3 Predictive Model

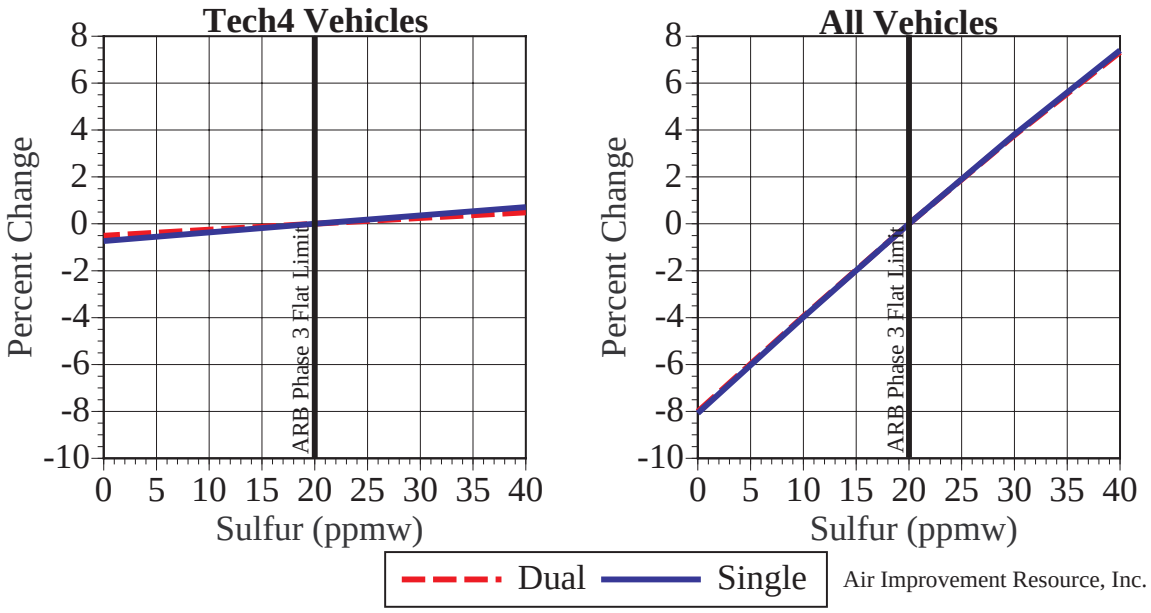


CO Emissions Percent Change from Reference Fuel vs Oxygen
ARB Draft3 Predictive Model



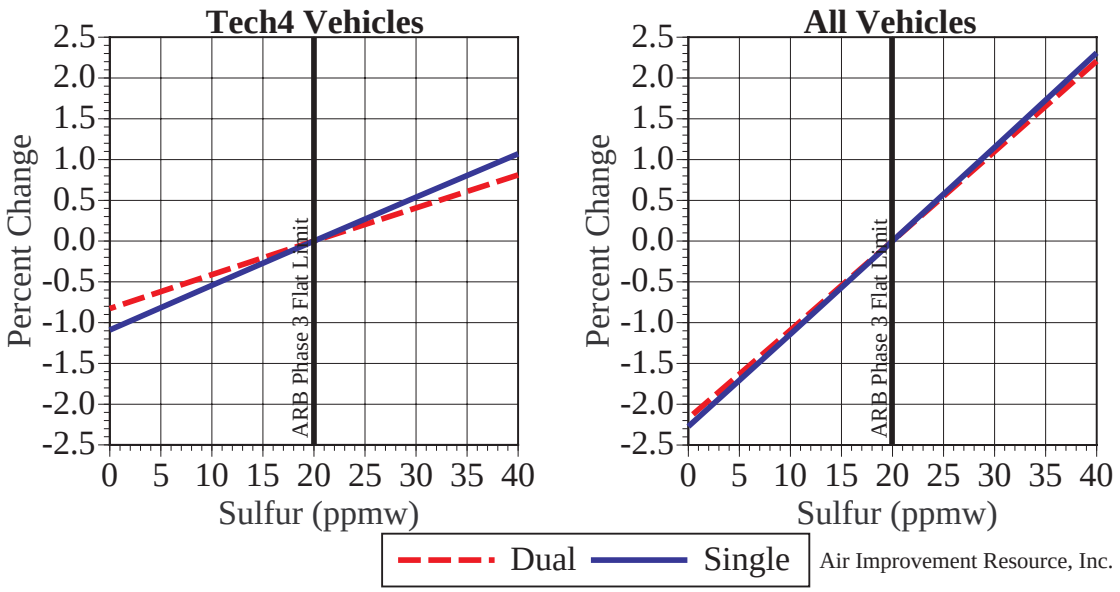
Air Improvement Resource, Inc.

NOx Emissions Percent Change from Reference Fuel vs Sulfur
ARB Draft3 Predictive Model

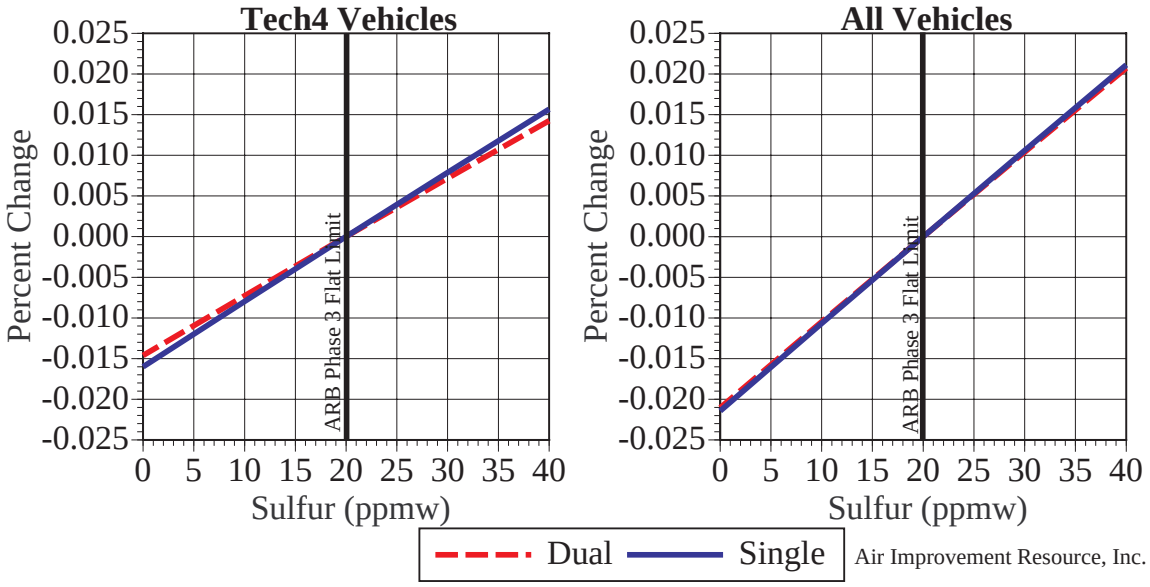


Air Improvement Resource, Inc.

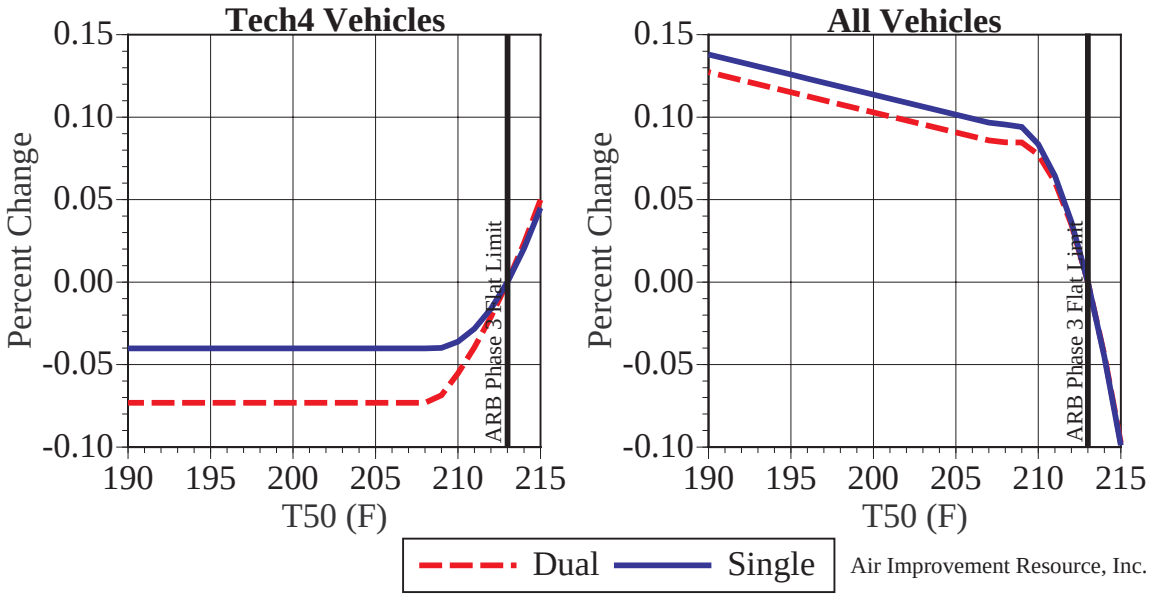
Exhaust THC Emissions Percent Change from Reference Fuel vs Sulfur
ARB Draft3 Predictive Model



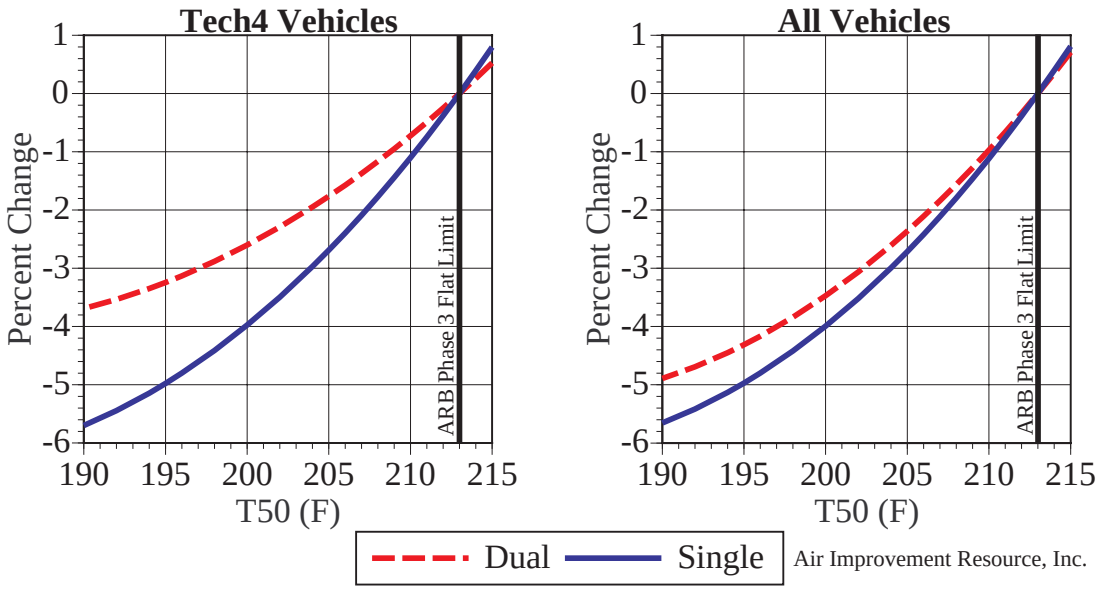
CO Emissions Percent Change from Reference Fuel vs Sulfur
ARB Draft3 Predictive Model



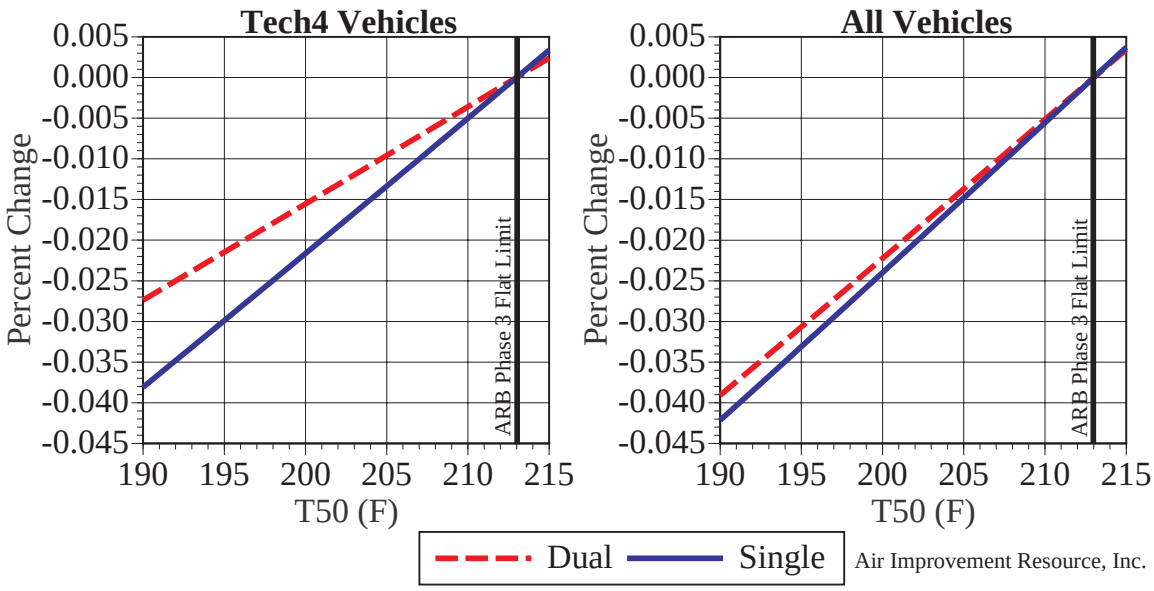
NOx Emissions Percent Change from Reference Fuel vs T50
ARB Draft3 Predictive Model



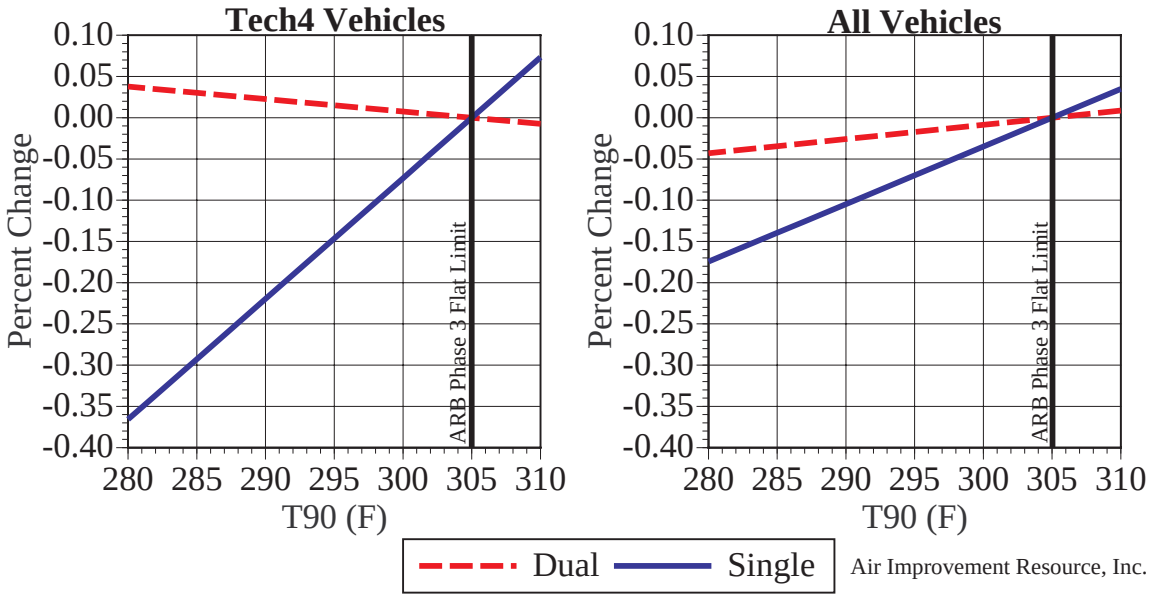
Exhaust THC Emissions Percent Change from Reference Fuel vs T50
ARB Draft3 Predictive Model



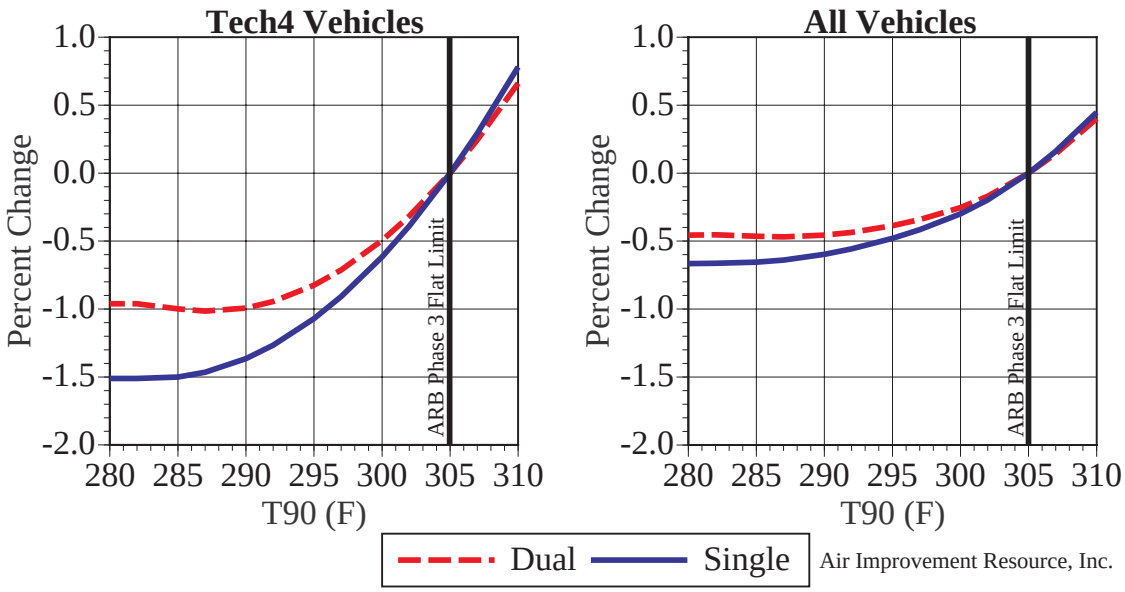
CO Emissions Percent Change from Reference Fuel vs T50
ARB Draft3 Predictive Model



NOx Emissions Percent Change from Reference Fuel vs T90
ARB Draft3 Predictive Model



Exhaust THC Emissions Percent Change from Reference Fuel vs T90
ARB Draft3 Predictive Model



CO Emissions Percent Change from Reference Fuel vs T90
ARB Draft3 Predictive Model