APPENDIX D
DATA AND STATISTICAL MODELS

CONTENTS

D-1) EXHAUST EMISSIONS MODELS– DESCRIPTION AND DERIVATION

A. BACKGROUND

The California Phase3 Reformulated Gasoline (CaRFG3) Predictive Model, adopted by the Board in 1999. The update from CaRFG2 Predictive Model was done to provide more flexibility for refiners to transition from the use of methyl-tertiary-butyl-ether (MTBE) oxygenate to ethanol while preserving the benefits of the CaRFG2 program. The updated model reflected more accurately changes in the vehicle fleet and incorporated data from the most recent vehicle/fuel emission test studies. A new technology group 'Tech 5' (1994-2005), Federal Tier I and California low-emission vehicles (LEVs), was added to the CaRFG3 Predictive Model. These vehicles employed improved emissions control technology compared to the 'Tech 4' vehicles (1986-1993). In addition, the new Predictive Model included an optional evaporative emissions module and allowed refiners to account for a carbon monoxide (CO) credit.

In the current update, staff proposes several changes to the current CaRFG3 Predictive Model to reflect the changes in vehicle fleet based on the ARB's latest motor vehicle emission inventory model EMFAC 2007. The update also provides an opportunity to include the results of recent emission test programs for Tech 5 with more advanced emissions control technology, such as ultra low emission vehicle (ULEV) and super ultra low emission vehicle (SULEV).

The new Predictive Model includes the following changes in the exhaust module:

<u>Database:</u>

- Condense the database by averaging the repeats
- Add Tech 5 vehicles data
- Change Tech 4 and Tech 5 definitions
- Add high influence tests data previously excluded

<u>Modeling Approach:</u>

- No RVP interaction terms allowed (Tech 3-5)
- Limit adjustment terms to those supported by recent studies (Tech 5)
- Maintain statistical hierarchy (Tech 5)

<u>New Exhaust Models:</u>

- Build stand alone CO model (Tech 3-5)

This Appendix describes the procedures used to develop the model for hydrocarbons (THC), oxides of nitrogen (NOx), and carbon Monoxide (CO). In every step of the model development, staff consulted with the statistical working group that consisted representatives from oil, car, and ethanol industries. Staff conducted regular meeting to discuss the working progress and to incorporate any suggestions from the group, regarding the appropriateness of the modeling approach being taken.

B. Database

The new test data have facilitated enhancement to the existing Tech 5 model, particularly the addition of test data for more advanced emission control technologies (ULEV and SULEV). These technologies will represent the majority of vehicle activities (population and vehicle miles traveled) in the future. Table 1 lists the new Tech 5 studies, including the number of observations, number of vehicles, and fuel properties tested.

Table 1
Summary of New Tech 5 Data

Study*	Fuel Prop Tested	# Fuels	# Veh	Emission Control Tech	# Obs
AAM/AIAM/Honda	Oxygen, Sulfur	6	13	TLEV, LEV, PULEV, ULEV	323
Toyota	Oxygen	2	9	TLEV, LEV ULEV	33
CRC E-60	Sulfur	3	14	LEV, ULEV, SULEV	201
CRC E-67	Oxygen, Distillation Temp (T50, T90)	12	12	LEV, ULEV, SULEV	326
ExxonMobil	Oxygen	4	5	LEV, ULEV	42
				T o t a l	925

*References 1-5 at the end of this Appendix

In addition to more than 9,000 data points existed in the current database, about 900 data points were added into Tech 5. About 100 observations from several studies involving high influence Tech 4 vehicles were excluded from the current database as suggested by the stakeholders when CaRFG3 was developed. The inclusion of these data produced unexpected response functions. The statistical working group proposed these data be included. This brings the total observations in the database to about 10,000.

Concerned with a serial correlation among observations resulted from non-randomized tests within a study, the working group proposed to represent multiple emission measurements from the same vehicle/fuel combination with its average emissions. This averaging was also expected to eliminate the unexpected response in Tech 4 model as briefly discussed above. As a result, the condensed database reduced the number of observations by 40 percent, from about 10,000 to 6,000 observations.

Staff redefined Tech 4 and Tech 5 groups in the new Predictive Model. In the current model, the 1994-1995 vehicles were assumed to represent Tech 5 prototype vehicles. Upon further consideration, the working group recommended these vehicles be

reclassified as Tech 4. Table 2 compares vehicle technology classification by model year between the current and proposed new models.

Table 2
Vehicle Classification by Model Year

Vehicle Class	Current Model	Proposed New Model
Tech 3	MY 1981-1985	MY 1981-1985
Tech 4	MY 1986-1993	MY 1986-1995
Tech 5	MY 1994 or newer	MY 1996 or newer

C. STATISTICAL MODELS:

The main objective of statistical modeling approach is to find a relationship between emissions (dependent variables) and fuel properties (independent variables) by technology group and pollutant, as follows:

$$\mathbf{y}_{p,t} = \beta_0 + \beta_1\mathbf{x}_1 + \beta_2\mathbf{x}_2 + \beta_3\mathbf{x}_3 + ... + \beta_n\mathbf{x}_n + \boldsymbol{\varepsilon}$$

where,

$\mathbf{y}_{p,t}$ (vector) = measured emission for pollutant, p, from vehicles in tech group, t
β_i = parameter to be estimated from the data
$\mathbf{x}_i$ (vector) = fuel property
$\boldsymbol{\varepsilon}$ (vector) = error term

The term 'linear' stems from the fact that the dependent variable is linearly related to fuel properties through β's (model parameters).

1. Mixed Models

The Predictive model database was collected from a random sample of on-road vehicles tested on narrowly varied fuel parameters. The modeling results are used to make inference on a wide variety of gasoline blends that meet the California reformulated gasoline standards for the whole vehicle population. In this model development vehicles are considered the random effects while fuel effects are considered fixed. Having both random and fixed effects in the same linear model is referred to as a mixed effects model.
In contrast, only fixed effect is considered in a classical regression model. In this report, SAS version 9.1 of the SAS Institute's statistical software was used to estimate the model coefficients.

2. Forward-Stepwise Regression

The independent variables are not limited to seven linear or first-order terms of fuel properties: Reid's vapor pressure (RVP), distillation temperatures (T50 and T90),

aromatics (ARO), olefins (OLE), oxygen (OX), and sulfur (S) content. They may also include 28 interaction terms (e.g., OX*OX, ARO*OX, etc.), where one fuel property is paired with itself (squared term) or another property (cross term), so a total of 35 possible independent variables exists. Unlike interaction terms that are added to the model when they are significant predictors, the linear terms are always present in the model.

The forward-stepwise regression to select the most significant variable to enter the model follows the same approach taken in the previous model. The stepwise procedure starts out with seven linear terms which then adds each of the remaining 28 terms one at a time. At the end, the most significant variable based on t-statistics will be added the model. This variable selection is repeated until there is no more significant variable that can be included. However, at any stage when a variable is found not significant upon adding another, this variable is removed from the model. The removed variable is potentially reselected at later steps.

3. Random Balance

The working database to build the Predictive Model includes wider range of fuel properties (fuel box) than is allowed by the California reformulated gasoline standards. As a result, the 'raw' models that are developed over a wider fuel box may include second-order terms that do not contribute to the predictive power over a smaller fuel box. For example, a quadratic term could be represented by a straight line over a small range of fuel property. This will result in a simpler model.

The working group recommended that staff use the same 'random balance' technique, developed by Dr. H. T. Mc Adams of the Advanced Computing Center of Argenta, to simplify the model. Table 3 shows the reformulated gasoline fuel box for the random balance procedure. The fuel properties are practically the same as the current model's, except for sulfur that was lowered to 20 from 30 ppmw.

D. REGRESSION EQUATIONS BY VEHICLE TECH CLASS

The comparison of regression equations by tech class and pollutant for the current and new models are discussed in the following paragraphs. The emphasis is on the second-order terms since all models contain the seven linear terms. Staff had consulted with stakeholders regarding RVP interaction terms (e.g., RVP*RVP, RVP*OX, etc.) as candidate variables in the stepwise procedure. RVP is one single fuel property that is highly correlated with others, and most of the studies in the database did not explicitly control fuel volatility in their tests. As a result, the inclusion of RVP interaction terms in a model tends to result in unexpected response function. Because of this intractable result, staff reached a consensus with stakeholders to limit RVP interaction terms from entering the model.

Table 3
Fuel Properties Range ('Box')
For Random Balance Procedure

Fuel Property	Unit	Lower Limit	Upper Limit
Aromatic Hydrocarbons (ARO)	% vol.	10	35
O l e f i n s (OLE)	% vol.	0	10
O x y g e n (OXY)	% wt.	0	3.5
Reid Vapor Pressure (RVP)	psi	6.4	7.2
S u l f u r (S)	ppmw	0	20
50% Distillation Temp (T50)	deg. F	160	220
90% Distillation Temp (T90)	deg. F	260	330

1. Technology Group 3

Since no new observations were added to Tech 3 class database, no significant change is expected from condensing the database. Tables 4-5 show the new Tech 3 THC and NOx models, respectively, including the current models coefficients while Table 6 shows the new CO model. As can be seen from the tables, both new and current models of THC and NOx are comparable.

2. Technology Group 4

Tech 4 database includes vehicles (MY 1993-1994) that were previously considered as Tech 5 prototypes. In addition, high influence vehicles data that were deleted in the current model were put back to the database. Table 7 shows high influence vehicles, about 100 observations, removed from the current Tech 4 database.

Stakeholders proposed to construct Tech 4 NOx high emitter model separately, using either 1 or 0.6 times of NOx emissions standard (1 gram/mile) as the dividing line (See References 6-7). Those emitting above the threshold were considered high emitter vehicles. This required bifurcation of Tech 4 database that would result in overall better model's fit (i.e., higher log-likelihood value). Staff investigated this issue from both technical and statistical aspects.

From the technical point of view, staff focused on the appropriateness of choosing 1 or 0.6 times of NOx emissions standard as a threshold for classifying high emitter vehicles. Staff consulted with representatives of the ARB's Mobile Source Control Division (MSCD) and those from the Alliance of Automobile Manufactures (AAM), as well as the Association of International Automobile Manufacturers (AIAM) to discuss this subject.

Table 4
Tech Class 3
Hydrocarbons Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Current Model		New Model	
	R a w	Random Balance	R a w	Random Balance
Intercept	-0.77651	-0.79147	-0.779100	-0.752270
RVP	0.00044	0.00047	-0.000030	-0.000005
T50	0.01112	0.01086	0.015860	0.015847
T90	0.01253	0.00218	0.011740	0.011768
ARO	-0.03066	-0.04375	-0.016760	0.014103
OL	-0.01909	-0.03064	-0.016510	-0.016533
OX	-0.02688	-0.02688	-0.026360	-0.026365
SU	0.00531	0.00550	0.012030	0.038207
T90*ARO	0.01811		0.016600	0.016606
ARO*SU	-0.04563	-0.04566	-0.030170	
RVP*T50	-0.01742	-0.01748		
T90*OL	-0.00910		-0.008030	-0.007995
ARO*OL	0.00986			

Table 5
Tech Class 3
Oxides of Nitrogen Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Current Model		New Model	
	R a w	Random Balance	R a w	Random Balance
Intercept	-0.13660	-0.07943	-0.159800	-0.159800
RVP	-0.02792	0.01356	-0.016150	-0.016150
T50	-0.01002	-0.00983	-0.007360	-0.007360
T90	-0.00056	-0.00052	0.000654	0.000654
ARO	0.05314	0.05321	0.047060	0.047060
OL	0.02294	0.02302	0.021110	0.021110
OX	0.01728	0.01724	0.014910	0.014910
SU	0.01601	0.01594	0.028040	0.028040
T90*ARO	-0.00808	-0.00968		
T50*T90	-0.00971	0.00755		
RVP*T50	0.00754	-0.00801		
RVP*RVP	-0.00726			

Table 6
Tech Class 3
Carbon Monoxide Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	New Model	
	R a w	Random Balance
Intercept	1.588700	1.615613
RVP	-0.004620	-0.004594
T50	0.009907	0.009897
T90	-0.025460	-0.025449
ARO	0.054570	0.085541
OL	0.002466	0.002416
OX	-0.068980	-0.068986
SU	0.005579	0.031849
T50*T90	0.017460	0.017463
ARO*SU	-0.030280	

Table 7
Tech 4 High Influence Vehicles

Study	Vehicle ID	# Obs
ARBMSD96	All	21
CHEVOX99	All	32
ARBETOH	All	38
EPA_PH3	I	10
T o t a l		101

Staff learned that car manufactures do calibrate their vehicle emission control systems to emit at levels below the standards as a margin of safety of production. However, there is no technical reason to believe that car emitting just below the margin or slightly above the margin should behave differently when subjected to the same fuel property changes. Staff conducted sensitivity analyses, and concluded that the selection of threshold was arbitrary that would result in statistically over-fitted models. Each model, normal and high emitter, would fit the partitioned data exceedingly well. The drawback is that such models tended to produce inconsistent response when subjected to fuel property changes not seen in the dataset or when the threshold was slightly change.

In a Fuels Workshop, stakeholders pointed out that the draft NOx model, as shown in Table 8, contains unexpected responses with respect to olefins and aromatics. Figure 1

shows that the draft model is less sensitive to olefins changes than the current model while Figure 2 shows steeper response for aromatics less than 25 volume percent. Staff investigated this issue, and found that the unexpected results were caused by olefin squared terms. Removing this term also solved the unexpected aromatic results. Figures 3 and 4 show the revised NOx model is comparable to the current model. Tables 9-11 show the estimated coefficient of new THC, NOx, and CO models.

3. Technology Group 5

Although several new studies have increased the number of observations in Tech 5 dataset, these data were limited to the effect of certain fuel property changes, mostly sulfur and oxygen, on emissions. As a result, the new Tech 5 dataset does not support a stand alone model. Stakeholders concurred that Tech 5 vehicles are similar to Tech 4, so there was an agreement to nest Tech 5 within Tech 4. This means the databases of both technology groups are pooled together and all the terms derived from Tech 4 models (Tables 14 and 15) are retained. While Tech 5 might have different response to certain fuel properties than Tech 4, these differences were handled through the use of indicator
variables. The emphasis will be given to those fuel properties that were found to affect emissions on newer vehicle technologies. Table 11 shows Tech 5 adjustment terms and the studies that support the findings. The following equation describes the structure of the model, and a sample of SAS code, input, and output are attached at the end of this section:

$$\mathbf{y}_p = \beta_0 + \beta_1\mathbf{x}_1 + \beta_2\mathbf{x}_2 + \beta_3\mathbf{x}_3 + ... + \beta_n\mathbf{x}_n + \beta_{n+1}\mathbf{I} + \beta_{n+2}\,\mathbf{J}X.. + \beta_{n+J}\,\mathbf{K}Y + \boldsymbol{\varepsilon}$$

where

$\mathbf{y}_p$ (vector) = measured emission for pollutant, p, from Tech 4 and 5 vehicles
β_i = parameter to be estimated from the pooled data
$\mathbf{x}_i$ (vector) = fuel property with second-order terms as shown in Tables 14 15
I (vector) = indicator variable (zero if tech group is 4, one otherwise)
J, K (vector) = indicator variables (zero if the observation not from particular Tech 5 studies, one otherwise)
X and Y = fuel properties found to affect Tech 5 more than Tech 4, as described in Table 12
$\boldsymbol{\varepsilon}$ (vector) = error term

When the model is refitted to the pooled data, the intercept will be β_0 plus β_{n+1}; similarly, the coefficient for any other variable will be the sum of the Tech 5 adjustment term and the corresponding term from Tech 4.

Stakeholders proposed two options (Option 1 and 2) on how Tech 5 adjustment terms should be modeled. Staff investigated these proposals. The objective of these new approaches is to put less influence of Tech 4 dataset on Tech 5 model coefficients. However, the results show that the proposed methods gave similar Tech 5 emissions to the current method (Basecase), except for CO emissions to fuel sulfur content.

Figures 5 shows steep Tech 5 CO emissions change to sulfur of the new approaches relative to the basecase. Staff believed these results are not supported by any of the Tech 5 studies, so stakeholders agreed to use the basecase approach with a minor modification. The objective of this modified approach is to maintain a hierarchical structure of the model. This change involves the inclusion of a linear term to accompany any squared terms included in Tech 5 adjustment terms. Tables 13-15 show the modeling results of THC, NOx, and CO.

Table 8
Tech Class 4
Oxides of Nitrogen Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Draft Raw Model
Intercept	-0.635700
RVP	0.006125
T50	-0.001990
T90	0.002715
ARO	0.020290
OL	0.007241
OX	0.014130
SU	0.049870
OX*OX	0.010240
SU*OX	-0.013240
T50*T50	0.006487
SU*SU	-0.005480
OX*OX	0.009877
OL*OL	0.006300
AR*AR	-0.004410

Figure 1. Tech 4 NOx Response to Olefins
(All Other Fuel Properties @ Flat Limits)

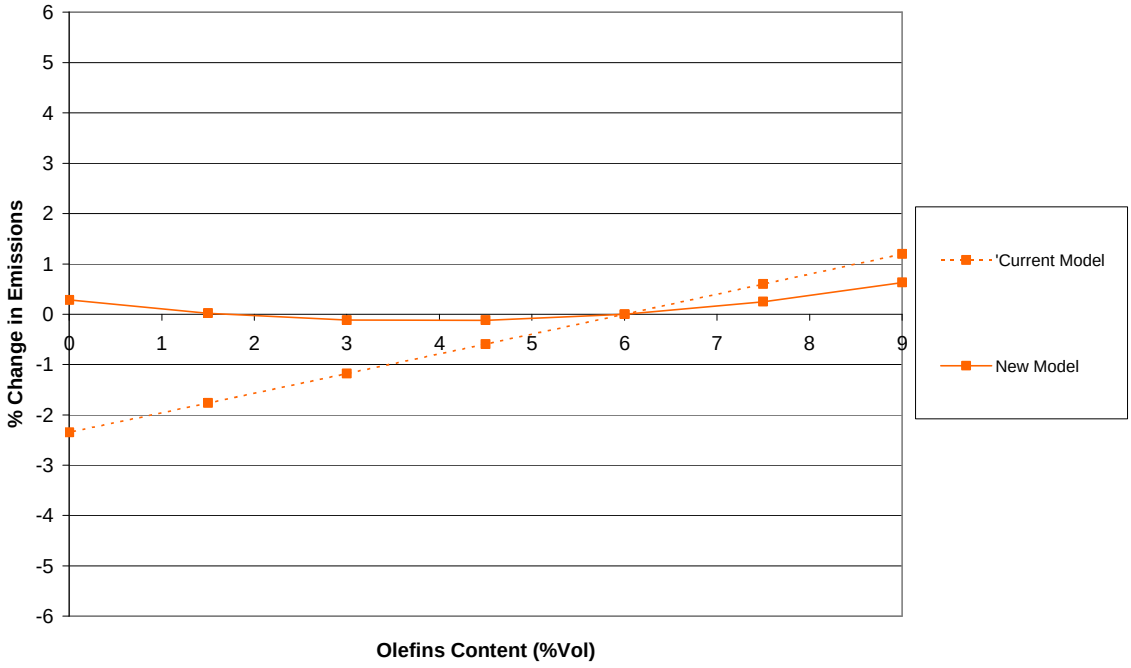

Figure 2. Tech 4 NOx Response to Aromatics
(All Other Fuel Properties @ Flat Limits)

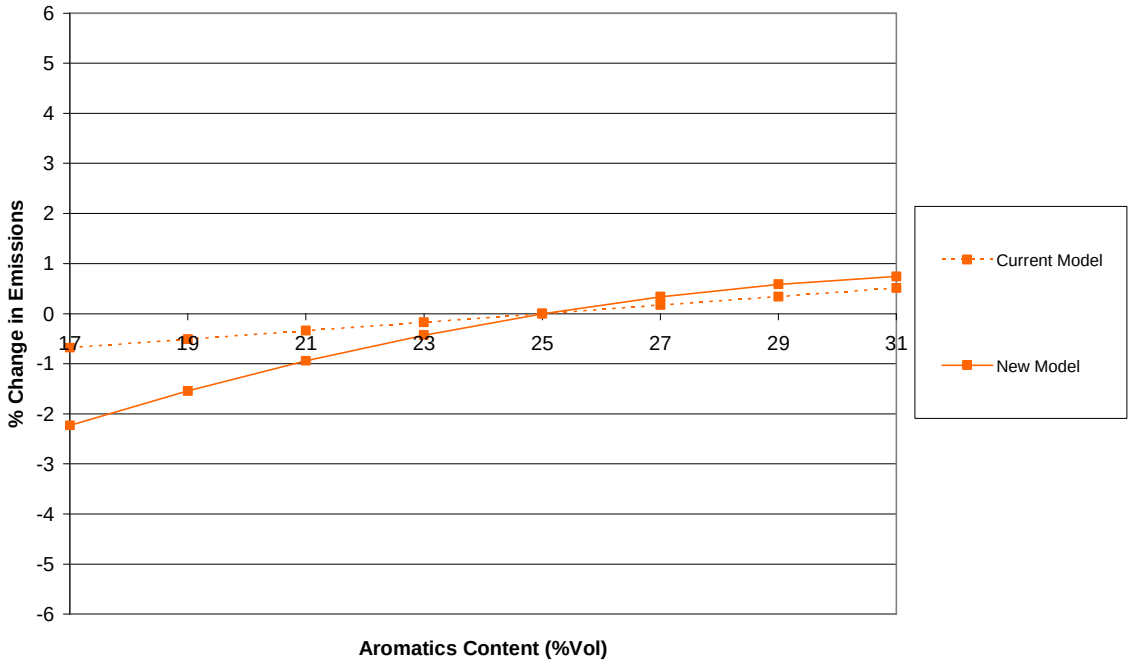

Figure 3. Tech 4 NOx Response to Olefins
(All Other Fuel Properties @ Flat Limits)

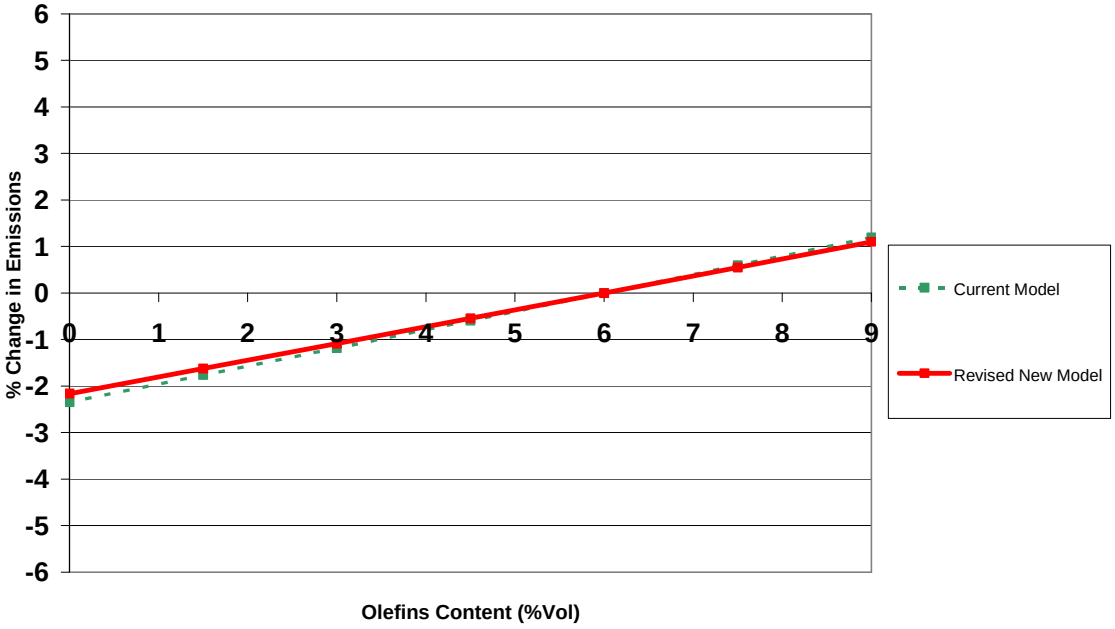

Figure 4. Tech 4 NOx Response to Aromatics
(All Other Fuel Properties @ Flat Limits)

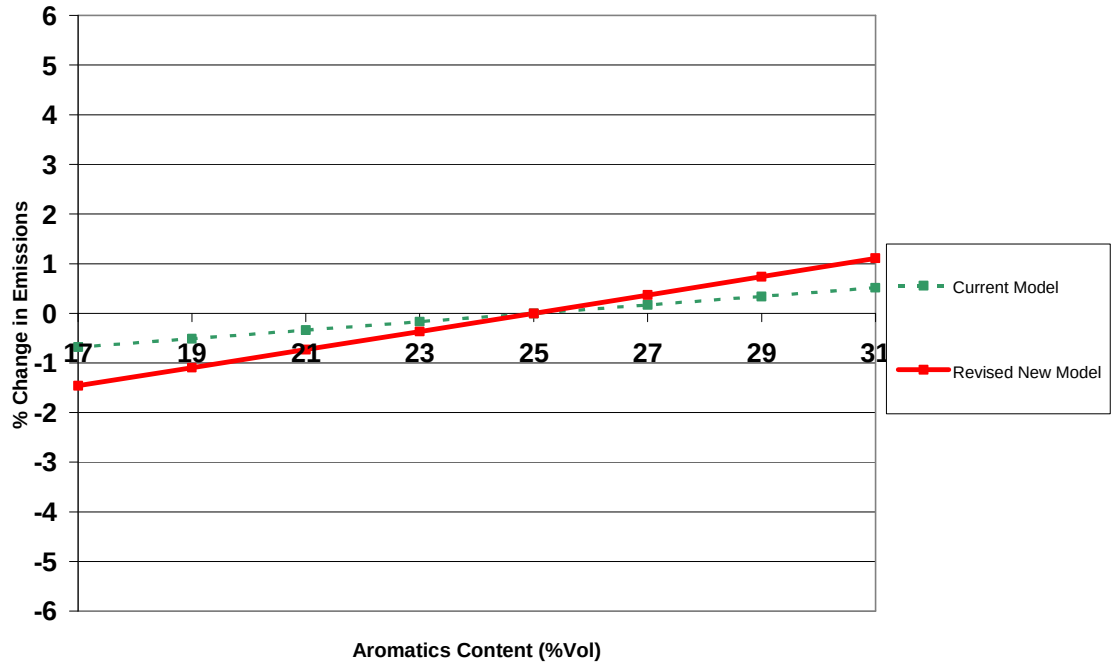

Table 9
Tech Class 4
Hydrocarbons Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Current Model		New Model	
	R a w	Random Balance	R a w	Random Balance
Intercept	-1.12820	-1.13142	-1.157800	-1.142182
RVP	0.01354	-0.01448	0.012580	0.012590
T50	0.06070	0.06068	0.052930	0.052939
T90	0.02745	0.04008	0.028060	0.037684
ARO	0.00011	0.00010	0.002043	0.002047
OL	-0.00936	-0.00938	-0.010720	-0.010716
OX	-0.01391	-0.01388	-0.019890	-0.019880
SU	0.06375	0.09279	0.056690	0.079373
T50*ARO			0.019030	0.019031
T50*T50	0.02011	0.02010	0.017080	0.017086
T50*OX			0.013720	0.013724
T90*ARO	0.00848	0.00847		
T90*OX	0.01046	0.01045		
T90*T90	0.01700	0.01699	0.013920	0.013914
ARO*ARO	-0.00861	-0.00860	-0.011000	-0.010999
ARO*OX			0.007222	0.007221
T90*SU	-0.01324		-0.009150	
SU*SU	-0.01057		-0.007460	
RVP*RVP	0.00873			

Table 10
Tech Class 4
Oxides of Nitrogen Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Current Model		New Model	
	R a w	Random Balance	R a w	Random Balance
Intercept	-0.59756	-0.60161	-0.633800	-0.634694
RVP	0.00640	0.00639	0.004547	0.004588
T50	-0.00020	-0.00020	-0.002430	-0.002431
T90	0.00556	-0.00055	0.002083	0.002087
ARO	0.00906	0.00905	0.017660	0.011366
OL	0.01847	0.01847	0.017180	0.017193
OX	0.01379	0.01378	0.014540	0.028711
SU	0.04745	0.04324	0.046710	0.051043
OX*OX	0.01024	0.01024	0.010720	0.010737
T50*T50			0.006274	0.006268
T90*ARO			-0.002890	-0.002892
SU*OX			-0.013460	
ARO*SU			0.005974	
SU*SU			-0.004990	
T90*SU	0.00640			
ARO*OX	-0.00587	-0.00587		

Table 11
Tech Class 4
Carbon Monoxide Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	New Model	
	R a w	Random Balance
Intercept	1.186300	1.195246
RVP	0.016850	0.016851
T50	0.022750	0.022750
T90	-0.008820	-0.008820
ARO	0.025960	0.025960
OL	0.001263	0.001263
OX	-0.052530	-0.052530
SU	0.056610	0.073616
SU*SU	-0.008070	
OX*OX	-0.016510	-0.016510
T50*ARO	0.009884	0.009884
T90*OL	-0.007360	-0.007360
T90*T90	0.007767	0.007767

Table 12
Tech 5 Adjustment Terms

Study*	Fuel Prop Tested
AAM/AIAM/Honda	OX, OX*OX, SU, SU*SU
Toyota	OX, OX*OX
CRC E-60	SU, SU*SU
CRC E-67	OX, OX*OX, T50, T50*T50, T90, T90*T90, T50*OX, T50*T90, T90*OX
ExxonMobil	OX, OX*OX

Figure 5. CO Response to Sulfur
(All Other Fuel Properties @ Flat Limits)

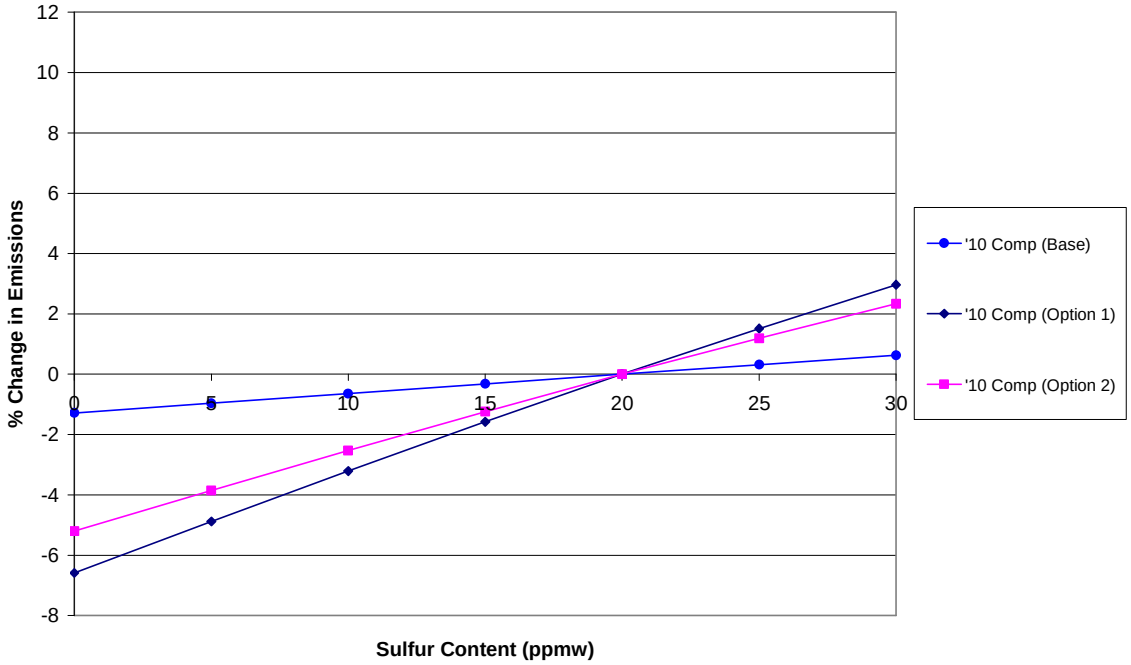

Table 13
Tech Class 5
Hydrocarbons Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Current Model		New Model	
	R a w	Random Balance	R a w	Random Balance
Intercept	-2.52154	-2.50695	-2.684300	-2.671187
RVP	0.01295	-0.01528	0.009470	0.009477
T50	0.05749	0.05747	0.056790	0.056796
T90	0.02796	0.03846	0.004280	0.010803
ARO	0.00098	0.00098	0.003037	0.003039
OL	-0.00965	-0.00968	-0.010910	-0.010908
OX	-0.01478	-0.01475	-0.007536	-0.007528
SU	0.18673	0.18673	0.219390	0.242238
T50*ARO			0.016760	0.016761
T50*T50	0.01906	0.01905	0.019560	0.019563
T50*OX			0.011594	0.014082
T90*ARO	0.00883	0.00882		
T90*OX	0.01015	0.01015	0.013370	0.013372
T90*T90	0.01653	0.01652	0.015220	0.015216
ARO*ARO	-0.00863	-0.00862	-0.009740	-0.009740
ARO*OX			0.006902	0.006902
T90*SU	-0.01101		-0.006840	
RVP*RVP	-0.03183			
SU*SU	0.00880		-0.009540	

Table 14
Tech Class 5
Nitrogen Oxides Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	Current Model		New Model	
	R a w	Random Balance	R a w	Random Balance
Intercept	-1.78141	-1.72822	-2.177300	-1.599255
RVP	0.00679	0.00680	0.000300	0.000394
T50	-0.00148	-0.00148	0.012400	0.012397
T90	0.00353	-0.00477	0.000800	0.000762
ARO	0.01013	0.01012	0.013700	0.013671
OL	0.01883	0.01883	0.017300	0.017335
OX	0.01373	0.01371	0.006300	0.016036
SU	0.31524	0.43284	-0.265500	0.947915
T50*T50			-0.022200	-0.022211
T50*OX			-0.015600	-0.015564
SU*OX			-0.010200	
T90*SU	0.00868			
SU*SU	-0.06438		-0.635800	
OX*OX	0.01013	0.01013	0.015200	0.015199
ARO*OX	-0.00592	-0.00592		

Table 15
Tech Class 5
Carbon Monoxide Models
Summary of Model Coefficients in the Regression Equations

Second-Order Term	New Model	
	R a w	Random Balance
Intercept	-0.258600	-0.240521
RVP	0.010720	0.010447
T50	0.018150	0.018195
T90	-0.120020	-0.128296
ARO	0.025600	0.025775
OL	-0.000030	0.005001
OX	-0.088040	-0.087967
SU	0.096640	0.123649
SUSU	-0.012530	
OXOX	0.026380	0.026309
T5AR	0.009802	0.009797
T9OL	-0.007630	
T9T9	0.007764	
T5OX	0.021700	0.021763

ATTACHMENT

Tech 5 CO
Input, Output, and Stepwise Regression SAS codes:

INPUT:

```
FILENAME IN1 DDE 'Excel|C:\Database
PM\[PM_Database_2006_Condensed.xls]Condensed Database!R2C1:R5824C25' NOTAB;
LIBNAME Tech 'C:\Win\Input\';
TITLE1 'PM Condensed Database 2006';
DATA Tech.CONDENSED;
   INFILE IN1 lrecl=8000 firstobs=1 DLM='09'X MISSOVER DSD ;
   INPUT STUDY $ VEHICLE $ FUEL $ MODEL_YR DRYBULB NOX CO THC
      NMHC AR BENZ ETBE ETOH MTBE TAME OL OX RV
      SU T5 T9 EXBENZ EX13BUTD EXFORMAL EXACTALD;
run;
DATA CONDENSED ; SET Tech.CONDENSED ;

/* TECH GROUPS DEFINITION */
IF MODEL_YR EQ ' ' THEN TECH = 5;
   ELSE IF MODEL_YR LT 1986 THEN TECH = 3;
   ELSE IF MODEL_YR LT 1996 THEN TECH = 4;
   ELSE TECH = 5;

/* CREATE NEW VARIABLES */
LN_THC = LOG (THC);
LN_NOX = LOG (NOX);
LN_CO  = LOG (CO);
NEW    = STUDY||VEHICLE;

/* TECH GROUPS SELECTION */
IF TECH = 4 OR TECH = 5;

RUN;
PROC STANDARD MEAN=0 STD=1 DATA=CONDENSED OUT=TEMP000 PRINT;
TITLE1 "TECH 4 AND 5 POOLED DATA";
TITLE2 "FUEL PROPERTY MEANS AND STANDARD DEVIATIONS";
VAR RV T5 T9 AR OL SU OX BENZ;
RUN;
DATA Tech.GROUP_5;
    SET TEMP000;
    /* INTERACTION TERMS */
        RVRV=RV*RV;
        RVT5=RV*T5;
        RVT9=RV*T9;
        RVAR=RV*AR;
        RVOL=RV*OL;
        RVSU=RV*SU;
        RVOX=RV*OX;
             T5T5=T5*T5;
             T5T9=T5*T9;
             T5AR=T5*AR;
             T5OL=T5*OL;
             T5SU=T5*SU;
             T5OX=T5*OX;
        T9T9=T9*T9;
        T9AR=T9*AR;
        T9OL=T9*OL;
```

```
        T9SU=T9*SU;
        T9OX=T9*OX;
             ARAR=AR*AR;
             AROL=AR*OL;
             ARSU=AR*SU;
             AROX=AR*OX;
        OLOL=OL*OL;
        OLSU=OL*SU;
        OLOX=OL*OX;
             SUSU=SU*SU;
             SUOX=SU*OX;
        OXOX=OX*OX;

     /* INDICATOR VARIABLE FOR TECH 5 (ALL)*/
        IF TECH=5 THEN I5=1;
        ELSE I5=0;

     /* INDICATOR VARIABLE FOR TECH 5 (AAMSUOXY, CRC_E67, EXXONMOB, AND
TOYOTA)*/
            IF TECH=5 & STUDY='AAMSUOXY' THEN J5=1;
               ELSE IF TECH=5 & STUDY='CRC_E67' THEN J5=1;
               ELSE IF TECH=5 & STUDY='EXXONMOB' THEN J5=1;
               ELSE IF TECH=5 & STUDY='TOYOTA' THEN J5=1;
               ELSE J5=0;

     /* ADJUSTMENT TERMS FOR TECH 5 (AAMSUOXY, CRC_E67, EXXONMOB, AND
TOYOTA)*/
        J5_OX=J5*OX;
        J5_OXOX=J5*OXOX;

      /* INDICATOR VARIABLE FOR TECH 5 (AAMSUOXY AND CRC_E60)*/
            IF TECH=5 & STUDY='AAMSUOXY' THEN K5=1;
               ELSE IF TECH=5 & STUDY='CRC_E60' THEN K5=1;
               ELSE K5=0;

     /* ADJUSTMENT TERMS FOR TECH 5 (AAMSUOXY AND CRC_E60)*/
        K5_SU=K5*SU;
        K5_SUSU=K5*SUSU;

     /* INDICATOR VARIABLE FOR TECH 5 (AAMSUOXY)*/
            IF TECH=5 & STUDY='AAMSUOXY' THEN L5=1;
               ELSE L5=0;

     /* ADJUSTMENT TERMS FOR TECH 5 (AAMSUOXY)*/
        L5_SUOX=L5*SUOX;

       /* INDICATOR VARIABLE FOR TECH 5 (CRC_E67)*/
            IF TECH=5 & STUDY='CRC_E67' THEN M5=1;
            ELSE M5=0;

     /* ADJUSTMENT TERMS FOR TECH 5 (CRC_E67)*/
        M5_T5=M5*T5;
        M5_T9=M5*T9;
            M5_T5T5=M5*T5T5;
            M5_T5T9=M5*T5T9;
            M5_T5OX=M5*T5OX;
        M5_T9T9=M5*T9T9;
        M5_T9OX=M5*T9OX;

RUN;
```

STEPWISE REGRESSION:

```
libname tech "C:\WIN\Input";
libname out "C:\WIN\Output";
OPTIONS LS=80 CLEANUP;
proc datasets library=out;
delete summary_1;
run;

%macro stepwise(techgrp,step,depvar,addterm);
      proc mixed data=&techgrp maxiter=500 method=reml noclprint;
            class new;
            title "Iter #&step (&addterm): &techgrp &depvar Model";
      model LN_&depvar = rv t5 t9 ar ol ox su
                                 susu oxox t5ar t9ol t9t9
                                 i5 m5_t9 j5_oxox m5_t5ox j5_ox m5_t5 /*the
last 2 added for hierarchy*/
                        &addterm
                        /s ddfm=res;
    random              int rv t5 t9 ar ol ox su
                                 susu oxox t5ar t9ol t9t9
                                 i5 m5_t9 j5_oxox m5_t5ox j5_ox m5_t5 /*the
last 2 added for hierarchy*/
                        &addterm
                        /sub=new;
      ods output solutionf=temp;
      run;

      data temp;
            set temp;
            length iter $ 5;
            iter="&step";
            abs_t=abs(tvalue);
            if upcase(effect)=upcase("&addterm") & abs_t>=1.96;
      run;

      proc append base=out.summary_1 data=temp;
      run;
%mend stepwise;

%macro call(techgrp,depvar);
    %stepwise(Tech.Group_5,00,CO,);
*    %stepwise(Tech.Group_5,01,CO,I5);
*    %stepwise(Tech.Group_5,02,CO,J5_OX);
*    %stepwise(Tech.Group_5,03,CO,J5_OXOX);
    %stepwise(Tech.Group_5,04,CO,K5_SU);
    %stepwise(Tech.Group_5,05,CO,K5_SUSU);
/*    %stepwise(Tech.Group_5,06,CO,L5_SUOX); */
*    %stepwise(Tech.Group_5,07,CO,M5_T5);
*    %stepwise(Tech.Group_5,08,CO,M5_T9);
    %stepwise(Tech.Group_5,09,CO,M5_T5T5);
/*    %stepwise(Tech.Group_5,10,CO,M5_T5T9); */
*    %stepwise(Tech.Group_5,11,CO,M5_T5OX);
    %stepwise(Tech.Group_5,12,CO,M5_T9T9);
    %stepwise(Tech.Group_5,13,CO,M5_T9OX);

      proc means data=out.summary_1 noprint;
            id abs_t;
```

```
            output out=maxinfo maxid(abs_t(abs_t iter effect)) = Max_abst
Iter Effect;
      run;

      data maxinfo;
            set maxinfo;
            drop abs_t _type_;
            rename _freq_=SignificantTerms;
      run;

      proc print data=maxinfo;
            title "Summary of &techgrp &depvar Model Added Term";
      run;
%mend call;

      %call(Tech.Group_5,CO)
```

OUTPUT:

```
                    Iter #00 (): Tech.Group_5 CO Model                    24
                                                 18:18 Wednesday, April 25, 2007

                           The Mixed Procedure

                            Model Information

            Data Set                      TECH.GROUP_5
            Dependent Variable            LN_CO
            Covariance Structure          Variance Components
            Subject Effect                NEW
            Estimation Method             REML
            Residual Variance Method      Profile
            Fixed Effects SE Method       Model-Based
            Degrees of Freedom Method     Residual


                               Dimensions

                     Covariance Parameters            20
                     Columns in X                     19
                     Columns in Z Per Subject         19
                     Subjects                       1036
                     Max Obs Per Subject              32


                          Number of Observations

                  Number of Observations Read           4971
                  Number of Observations Used           4971
                  Number of Observations Not Used          0


                            Iteration History

          Iteration    Evaluations    -2 Res Log Like       Criterion

                  0              1     12383.56816233
                  1              4      3053.97367306       .
                  2              3      3053.23356442       .
                  3              3      3053.22214731       .
                  4              3      2740.72925232       .
                  5              3      2699.61182720       .
                  6              3      2697.21321829       .
                  7              3      2691.54509256       .
                  8              3      2678.40591423       .
                  9              3      1947.49961241       .
                 10              3      1878.63157946       .
                 11              1      1442.00390834       .
                 12              1      1202.91709856       .
                 13              1      1103.83088328       .
                 14              1      1075.95168220       .
                 15              2      1068.54796693       .
                 16              3      1064.57081610       .
```

The Mixed Procedure

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
17	2	1063.91015401	.
18	1	1063.86632140	0.00000011
19	1	1063.86586045	0.00000000

Convergence criteria met.

Covariance Parameter Estimates

Cov Parm	Subject	Estimate
Intercept	NEW	0.7344
RV	NEW	0.001219
T5	NEW	0.000752
T9	NEW	0.001804
AR	NEW	0.000154
OL	NEW	0
OX	NEW	0.004540
SU	NEW	0.005982
SUSU	NEW	0
OXOX	NEW	0
T5AR	NEW	0.000107
T9OL	NEW	1.58E-20
T9T9	NEW	0
I5	NEW	0
M5_T9	NEW	0.008475
J5_OXOX	NEW	0.002377
M5_T5OX	NEW	0.000708
J5_OX	NEW	0.004879
M5_T5	NEW	0.001950
Residual		0.02104

Fit Statistics

-2 Res Log Likelihood	1063.9
AIC (smaller is better)	1091.9
AICC (smaller is better)	1092.0
BIC (smaller is better)	1161.1

The Mixed Procedure

Solution for Fixed Effects

Effect	Estimate	Standard Error	DF	t Value	Pr > |t|
Intercept	1.1991	0.03008	4952	39.86	<.0001
RV	0.01072	0.006462	4952	1.66	0.0971
T5	0.02189	0.005472	4952	4.00	<.0001
T9	-0.01162	0.005260	4952	-2.21	0.0272
AR	0.02560	0.004148	4952	6.17	<.0001
OL	-0.00003	0.003171	4952	-0.01	0.9914
OX	-0.05146	0.004608	4952	-11.17	<.0001
SU	0.09664	0.007087	4952	13.64	<.0001
SUSU	-0.01253	0.002569	4952	-4.88	<.0001
OXOX	-0.01595	0.005501	4952	-2.90	0.0038
T5AR	0.009802	0.003343	4952	2.93	0.0034
T9OL	-0.00763	0.002276	4952	-3.35	0.0008
T9T9	0.007764	0.003201	4952	2.43	0.0153
I5	-1.4577	0.08073	4952	-18.06	<.0001
M5_T9	-0.1084	0.03109	4952	-3.49	0.0005
J5_OXOX	0.04233	0.01358	4952	3.12	0.0018
M5_T5OX	0.02170	0.01032	4952	2.10	0.0355
J5_OX	-0.03658	0.02142	4952	-1.71	0.0878
M5_T5	-0.00374	0.01848	4952	-0.20	0.8397

Type 3 Tests of Fixed Effects

Effect	Num DF	Den DF	F Value	Pr > F
RV	1	4952	2.75	0.0971
T5	1	4952	16.00	<.0001
T9	1	4952	4.88	0.0272
AR	1	4952	38.10	<.0001
OL	1	4952	0.00	0.9914
OX	1	4952	124.74	<.0001
SU	1	4952	185.92	<.0001
SUSU	1	4952	23.77	<.0001
OXOX	1	4952	8.40	0.0038
T5AR	1	4952	8.60	0.0034
T9OL	1	4952	11.25	0.0008
T9T9	1	4952	5.88	0.0153
I5	1	4952	325.99	<.0001
M5_T9	1	4952	12.16	0.0005
J5_OXOX	1	4952	9.72	0.0018
M5_T5OX	1	4952	4.42	0.0355
J5_OX	1	4952	2.92	0.0878
M5_T5	1	4952	0.04	0.8397

The Mixed Procedure

Model Information

Data Set	TECH.GROUP_5
Dependent Variable	LN_CO
Covariance Structure	Variance Components
Subject Effect	NEW
Estimation Method	REML
Residual Variance Method	Profile
Fixed Effects SE Method	Model-Based
Degrees of Freedom Method	Residual

Dimensions

Covariance Parameters	21
Columns in X	20
Columns in Z Per Subject	20
Subjects	1036
Max Obs Per Subject	32

Number of Observations

Number of Observations Read	4971
Number of Observations Used	4971
Number of Observations Not Used	0

Iteration History

Iteration	Evaluations	-2 Res Log Like	Criterion
0	1	12368.29096091	
1	4	3061.59904109	.
2	3	3060.37688973	.
3	3	2743.20577575	.
4	3	2711.14538598	.
5	3	2708.82029813	.
6	3	2708.28980057	467.06101510
7	3	2703.65747588	.
8	3	1946.02562134	.
9	3	1864.10928124	.
10	1	1423.27123569	.
11	1	1175.15816251	.
12	1	1068.99703807	.
13	1	1037.55402145	.
14	2	1028.70707188	.
15	3	1025.22145254	.
16	1	1024.81794351	0.00000264

References:

1. Alliance of Automobile Manufacturers (AAM) and Association of International Automobile Manufacturers (AIAM), Sulfur Oxygen Vehicle Emissions Test Program (2001).

2. Toyota Motor Co., Effects of Ethanol on Emissions of Gasoline LDVs (2000).

3. CRC Project No. E-60, The Effect of Fuel Sulfur on NH3 and Other Emissions from 2000-2001 Model Year Vehicles (2003).

4. CRC Project No. E-67, Effects of Ethanol and Volatility Parameters on Exhaust Emissions (2006).

5. ExxonMobil Research and Engineering Company, LEV/ULEV Gasoline Oxygenate Study (1999).

6. ICF Consulting Memo and Presentation (May, 2006).

7. ICF Consulting Memo and Presentation (September, 2006).

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D-2) STAKEHOLDERS' COMMENTS ON EXHAUST MODELS

D-2.1) ICF Consulting (May 11, 2006)

Table 1. Percentages of normal and higher emitting vehicles and datapoints, log-likelihoods, for different percentage cutoffs.

Percentage	Normal Emitters		Higher Emitters		Normal Emitters		-2*Log Likelihood	
Cutoff	Vehicles	Datapoints	Vehicles	Datapoints	% Vehicles	% Datapoints	iter	noiter
40	235	2113	623	4818	73	70	-6470.1	-6407.3
60	499	3915	359	3016	42	44	-6637.3	-6616.2
80	652	5241	206	1690	24	24	-6422.9	-6421.5
100	740	6002	118	929	14	13	-6208.5	-6208.5
120	790	6415	68	516	8	7	-6065.2	-6060.0
140	808	6558	50	373	6	5	-6004.1	-6007.7
160	817	6618	41	313	5	5	-5966.4	-5974.8
180	820	6624	38	307	4	4	-5947.1	-5956.1
200	827	6684	31	247	4	4	-5881.0	-5887.9
TOTAL	858	6931	858	6931				

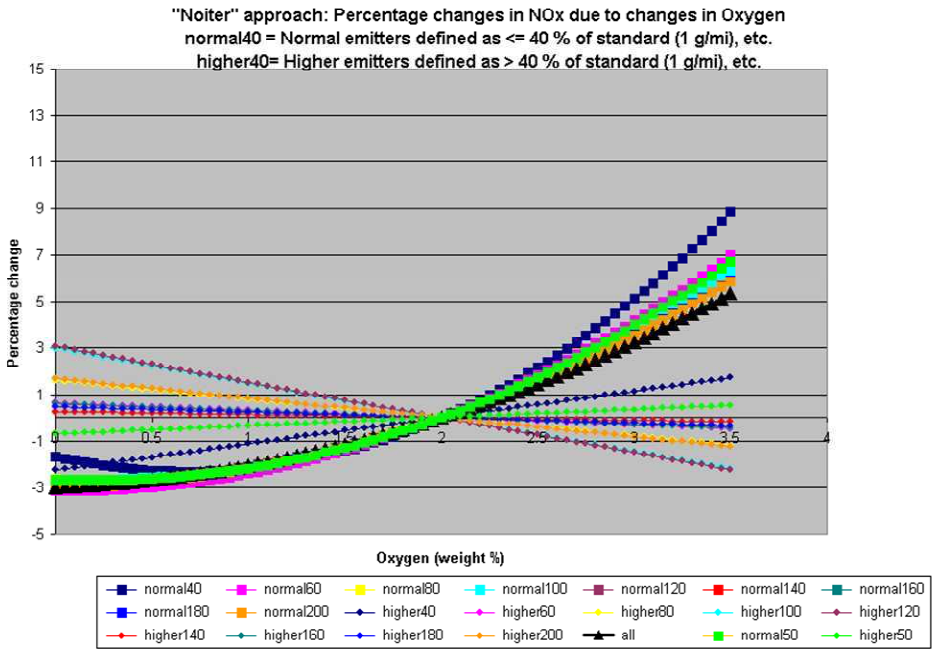


Figure 1. Percentage changes in NOx for different normal/higher emitter cutoffs using "noiter" approach, i.e., the same interactions as Version 2 for all models.

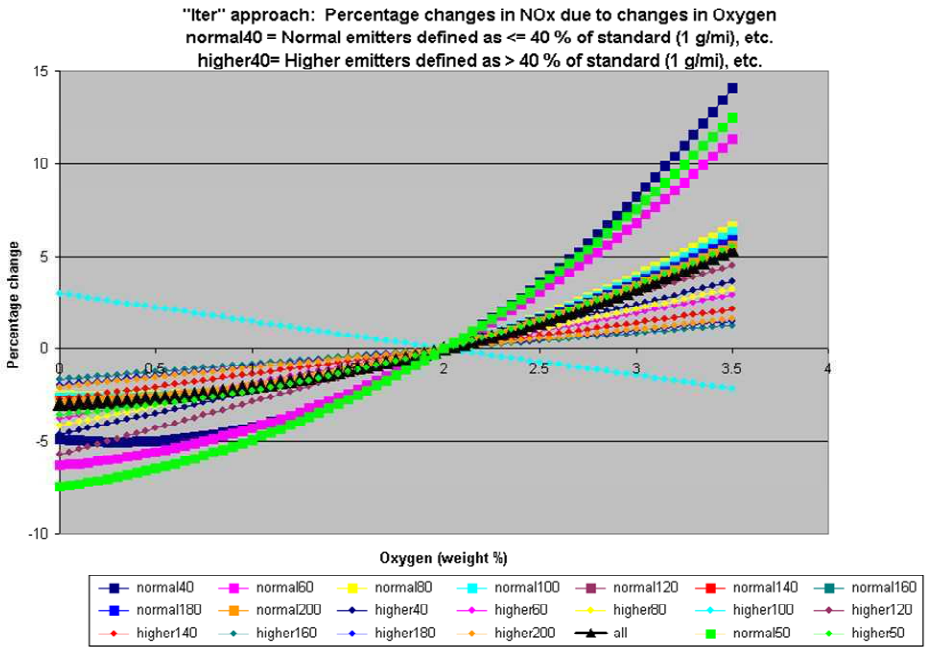


Figure 2. Percentage changes in NOx for different normal/higher emitter cutoffs using “iter” approach, i.e., interactions are selected using the iterative stepwise approach for all models.

D-2.2) Transportation Fuels Consulting Inc.

June 29, 2006

Mr. Dean Simeroth
Chief, Criteria Pollutants Branch
Stationary Source Division
California Air Resources Board
1001 I Street
P.O. Box 2815
Sacramento, CA 95812

Dear Mr. Simeroth:

I appreciate the opportunity to participate in the process of updating the Predictive Model, and the open process that you and your staff continue to employ.

I understand that stakeholders in the model update process have suggested that improvements in model performance could be realized by dividing the Tech 4 vehicle data set into two groups using a so-called dual model approach. A statistical analysis by Jonathan Cohen of ICF Consulting of NOx emissions performance vs. fuel oxygen content presented at the May 24, 2006 Predictive Model workshop in Sacramento suggested that the data fell into two separate populations; NOx emissions below 0.6 gm/mi, and NOx emissions higher than 0.6 gm/mi.

Based on my automotive emissions experience, I offer the following comments as a possible rationale for dividing the data set at a level less than the applicable Tier 0 federal NOx standard of 1.0 gm/mi.[1] Each vehicle-engine family configuration is designed by the manufacturers to perform at a level somewhat below the standard at its full useful life. This design target is chosen to accommodate the emissions performance variation inherent in the in-use vehicle population, and to insure compliance with the applicable standard. Although vehicle manufacturers do not publish their design targets, most fall within 50 to 75% of the standard.

As a result, a vehicle that is performing as designed could be expected to produce emissions levels at about 50-75% of the standard, or somewhat less depending on the vehicle mileage. So-called moderate emitters might have experienced several effects that increased their emissions to a level moderately higher than the standard (1-2 gm/mi). The emission control systems of vehicles in this category are likely to be fully functional, but somewhat compromised by either a small lean shift in air-fuel ratio which would reduce catalyst efficiency, or a loss in catalyst efficiency possibly caused by fuel poisoning, or thermal degradation.

[1] About 85 percent of the data is from LDVs certified to the 1.0 gm/mi standard, and the remainder is from light duty trucks certified to higher standards.

This loss in control system effectiveness may be due to improper use or maintenance, and the control system diagnostic "service engine" or "check engine" light may identify a component that is operating out of range. For example, a lean air-fuel ratio control shift can be caused by oxygen sensor poisoning or an exhaust system leak ahead of the catalyst. Catalyst thermal degradation can be a result of very aggressive driving, trailer towing or engine overheating.

Due to a compromised emission control system, the emission response of vehicles in the moderate emitter category to fuel oxygen is likely to be different than a normal emitter. Reduced catalyst efficiency resulting from a lean air fuel ratio shift or catalyst thermal degradation may be exacerbated by fuel oxygen under driving mode transients that are not effectively compensated by the control system, including possible catalyst break-through[2] and significantly higher tailpipe NOx emissions.

Ethanol blends have also been reported to reduce engine-out NOx due to lower combustion temperatures compared to gasoline without ethanol. The result of such competing effects on engine-out NOx are not easily predictable, and would depend on control system response and effectiveness. However, the effects of fuel oxygen are likely to be amplified by a compromised control system of moderate and higher emitter vehicles. It seems reasonable that modeling of moderate emitter vehicles separately from normal emitters might more accurately describe in-use emission performance. This rationale may not necessarily be applicable to Tech 5 or other vehicle categories due to several factors including OBDII systems which have been shown to improve in-use emission performance.

Although the level of 0.6 gm/mi determined by the statistical analysis of the data does not correspond exactly to a specific design target, it could represent a reasonable cut point between the normal and moderate emitter categories. Design targets for LDVs of 50 to 75% of the 1.0 gm/mi standard could range from 0.5 to 0.75. A simple average of that range is 0.62. Assuming that most manufacturers adopted targets closer to 50% of the standard, that level is likely to be reduced substantially below 0.62.

However, some data from light duty trucks contained in the database certified to the higher NOx standards of 1.2 gm/mi with design targets ranging from 0.6 to 0.9 could tend to increase the average design target level. The average design target might be in the range of 0.45 to 0.5. If it is assumed that the average design target represents a mean performance level of normal emitter vehicles at full useful life, the Tech 4 database mean for normal emitters should be somewhat lower due to vehicle test mileage at less than useful life. Then, it seems reasonable to assume that a large percentage of Tech 4 normal emitters would perform at well below the proposed 0.6 gm/mi cut point in the database.

[2]"Break-through" refers to a condition where catalyst conversion capacity is momentarily exceeded either by compromised catalyst performance or high engine out mass emissions, and conversion efficiency is very low.

Based on the foregoing discussion of emission control system performance, I can support the proposed dividing of the Tech 4 database above and below 0.6 gm/mi. I hope you will contact me directly with any questions, or if additional supporting information would be helpful.

Best regards,

Gary Herwick

D-2.3) ICF Consulting Inc. (September 18-22, 2006)

M E M O R A N D U M

To: California Air Resources Board

From: Jonathan Cohen

Date: 18 September, 2006

Re: Uncertainties of Oxygen-NOx effect from Predictive Model studies

The latest draft Predictive Model follows the same basic approach as the 1999-2000 CalRFG3 Predictive Model in that a statistical mixed model is fitted to all the studies in the database and the fixed effects component of that model is used to estimate the percentage changes in emissions due to changes in fuel properties from the base fuel. This approach is highly uncertain since it relies on the questionable assumptions that the combined set of test fleets is a random sample from the on-road fleet and that the fuel responses follow the fitted statistical model formulation. The assumption of a random sample is clearly invalid, as demonstrated by the severe under-representation of the EMFAC categories of moderate and higher NOx emitters. The uncertainty of the fitted model formulations is demonstrated in this memorandum by showing wide differences between predicted NOx effects due to oxygen for different studies and for different model formulations, with effects varying in direction (NOx increasing and decreasing with increased oxygen) and in statistical significance. Another major source of uncertainty for the Tech 4 and older vehicles is that many of the studies tested vehicles on fuels that are unrepresentative of current fuels, such as high sulfur or MTBE fuels, so that the statistical models have errors due to the extrapolation of these fuel properties to Phase 3 and later gasolines.

ICF previously presented to the ARB (e.g., August 2, 2005 Fuels Workshop presentation) an alternative approach to the Tech 4 model that addresses the uncertainty of the random sample assumption by using a dual model approach that separately fits statistical models to higher NOx emitters (emitting more than the 1 g/mile NOx standard) and normal emitters (emitting less than 1 g/mile NOx). More recently, ICF presented to the Predictive Model statistics workgroup, and to the ARB, variants of the dual model approach that redefine the higher emitter cutoff at different percentages of the standard, and found that the best-fitting models had cut-offs between 0.4 and 0.6 g/mile. In this memorandum we present results for the higher and normal emitter models using the three cutoffs 1 g/mile, 0.6 g/mile and 0.4 g/mile, the more recent Tech 4 database using averages across vehicle/fuel combinations, and the same five model formulations used to evaluate the individual studies. The higher emitter definition used here is based on the average emissions on the fuel closest to the Auto/Oil study fuel A, to address concerns that for some vehicles the average NOx across all fuels may bias the higher emitter results towards more higher-emitting fuels. As in the previous analyses, these dual models fit the data statistically significantly better than the single models do.

In view of the large uncertainties of the Predictive Model we believe that it is unrealistic to use the fixed effects from a single statistical model to precisely define compliance since these estimates do not address any of the uncertainties about the correct model formulation, about the representativeness of the data, and about the uncertainties of the predictions for the selected model. A more realistic, and more flexible approach would define compliance using the lowest lower confidence bound amongst several feasible competing statistical models, including the dual models described here.

The Database is Unrepresentative of the Emissions Distribution

A crucial assumption of the Predictive Model is that the database can be treated as if it were a random sample from the on-road fleet in the year to be modeled (currently assumed to be 2010). In fact the database consists of a compilation of various emissions studies over several years and no attempt has been made by the ARB to evaluate the representativeness of the data or to weight the data accordingly. This is a major source of uncertainty.

The database used for all the analyses in this memorandum is the latest version of the Predictive Model database published by the ARB on their website such that for each vehicle/fuel combination, the emissions are averaged over any multiple repeat tests, i.e., when the same vehicle/fuel combination is tested repeatedly. No averaging applies to the Tech 5 E-67 study, which used a different experimental design whereby each vehicle was tested once on all the test fuels and then the entire block of fuel tests was repeated in random order. The same vehicle tested in a different study is regarded as a different vehicle. No outliers are removed. The Tech groups are defined by the model years: Tech 3 = 1985 or earlier; Tech 4 = 1986-1995; Tech 5 = 1996 or later, including the Toyota and AAMSUOXY studies which were reported around 2000 but the vehicle model years were not provided to the ARB. These analyses focus on the NOx emissions for Tech groups 4 and 5.

To illustrate the lack of representativeness, consider the following two tables. Table 1 shows the numbers of observations (in most cases, vehicle/fuel combinations, with the exception of the E-67 study) from each model year and the percentages within each Tech group. For Tech group 4, the mode is at 1989, since a large percentage of the Tech 4 data is from the Auto/Oil study current fleet. For Tech 5, the mode is at 2003, but there are almost as many observations for 1997. The EMFAC model can provide detailed estimates of the model year distributions, but even without this information, common sense suggests that the on-road fleet will tend to be tilted more towards the more recent model years, unlike the pattern found in the ARB database.

Table 1. Number of Observations by Model Year			
Tech Group	Model Year	Obs	% of Tech Group
4	1986	659	16
4	1987	574	14
4	1988	438	10
4	1989	1632	39
4	1990	629	15
4	1991	77	2
4	1992	29	1
4	1993	13	0
4	1994	82	2
4	1995	52	1
5	1997	188	24
5	1998	4	1
5	1999	101	13
5	2000	18	2
5	2001	92	12
5	2002	58	7
5	2003	242	31
5	Unknown	83	11

Table 2 anticipates some of the later material in this memorandum concerning higher emitters. Using the definition d = 25 given below (the entire Tech 4 database) and a cutoff of 1 g/mi (100 % of the NOx standard) to define higher emitters, it shows that in the Tech 4 test fleet, 16 % of the observations, 13 % of the vehicles, and 38 % of the test fleet emissions are for higher emitters, but in the year 2005, the higher emitters in the California fleet emitted 79 % of the NOx. These calculations (from Graboski, Cohen and Pollack, 2000[3]) use the earlier EMFAC 2000 version of the EMFAC model and are based on the year 2005. More recent results using the latest EMFAC model for 2010 have not been made available but are expected to show a similar pattern of severely under-representing the higher emitters. In fact, since emissions tends to increase with vehicle age, one should expect the percentages of emissions attributable to higher emitter vehicles in 2010 to be greater than the estimates for 2005.

Table 2. Comparison of Test Fleet Tech 4 Normal and Higher Emitter Fractions with EMFAC 2000 Projections for 2005.						
Category	Obs	Obs	Vehicles	Vehicles	Emissions – Test Fleet	Emissions - EMFAC
	N	%	N	%	%	%
Normal	3535	84	779	87	62	21
Higher	650	16	121	13	38	79
Total	4185	100	900	100	100	100

[3] 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.*

These Tables demonstrate the lack of representativeness of the Predictive Model database for the distributions of model years (Table 1) and emissions (Table 2), showing that these data cannot reasonably be considered as a random sample from the on road fleet. The results would need to be confirmed by calculations using the latest version of the EMFAC model for the fleet and the emissions in the year 2010, but we would be surprised if the findings changed significantly.

If the NOx response to changes in the fuel parameters could be shown to be independent of model year and emissions level, then these results would be less important. However, while we have not evaluated the effect of model year, the analyses of the dual normal and higher emitter models presented below shows that the NOx response is statistically significantly different for different emissions levels, so that the bias of the test fleet data is a severe problem that should be addressed. The dual model approach is a recommended approach for addressing this problem, although it does not address all the problems with the database.

The Tech 4 Model Ignores the Uncertainties Due to Variation Within and Between Studies and Across Model Formulations

The ARB combined all the Tech 4 data and used a stepwise approach to fit a mixed model with fixed and random effects. There are seven fuel parameters: AR = aromatics, OL = olefins, OX = oxygen (weight percent), T5 = T50, T9 = T90, RV = RVP. The fixed effects are used to represent and estimate fleet average effects of changes in the seven fuel parameters on NOx. Each fixed effect is the fleet average value of a fuel parameter or interaction coefficient. The random effects represent the random variation of the coefficients across the vehicles in the California fleet, assumed to be normally distributed about the mean value (which is the fixed effect). The Predictive Model only uses the fixed effect values to predict NOx impacts.

The latest version of the ARB draft Tech 4 NOx model has all seven main effects plus the following seven interaction terms: OXOX, SUOX, T5T5, SUSU, OLOL, ARAR, ARSU. For example, OXOX is the square of the (normalized) oxygen term and SUOX represents SU times OX, i.e., the variation of the the oxygen effect with different levels of sulfur. To evaluate the consistency of the NOx model among the different studies, we fitted this model separately to each of the Tech 4 studies. The fuel parameters were renormalized to a mean of zero and a variance of 1 for each Tech group. Following the ARB approach, we used the method of restricted maximum likelihood (REML) to fit these and all the other models described in this memorandum (with the exception of the dual model significance tests described below). The difference between the REML and maximum likelihood (ML) fitted models is usually negligible although using the ML approach is necessary when comparing the goodness-of-fit of two different models with different random effects terms.

To evaluate how the uncertainty about the true statistical model leads to uncertainty in the predictions, we also compared this model, which we refer to as Model 5, with four simpler models, defined as follows:

- Model 1. Main term OX. Up to six additional linear terms. No interactions.
- Model 2. Main term OX. Up to six additional linear terms. Interaction term OXOX.
- Model 3. Main term OX. Up to six additional linear terms. Interaction term SUOX.
- Model 4. Main term OX. Up to six additional linear terms. Interaction terms OXOX and SUOX.
- Model 5. ARB Model. All seven linear terms. Interaction terms OXOX, SUOX, T5T5, SUSU, OLOL, ARAR, ARSU.

All of these models have the linear term OX, so that in most cases the effect on NOx of changing oxygen from 2 to 3.5 %, keeping all other fuel parameters at their base levels, can be estimated. The other six linear terms (and the interactions) adjust for the effects of the other fuel parameters. For Models 1, 2, 3, and 4 we used as many linear terms as possible as long as there were sufficient degrees of freedom to estimate the effect of changing oxygen from 2 to 3.5 % for the given data subset (e.g., a Tech 4 study). To do this, for each subset we calculated the coefficient of variation (CV = standard deviation divided by mean) for all six fuel parameters other than oxygen and then added them to the model in turn, starting with the parameter that had the greatest CV and then adding the parameter with the next highest CV, and so on. The main difference between Models 1, 2, 3 and 4 is whether we included one or both of the two OX interaction terms OXOX and SUOX; we tried to include these terms since they were the two OX interactions in the ARB models and their inclusion or exclusion is expected to impact the predicted NOx effect. The oxygen-NOx predictions tend to be most sensitive to whether or not the OXOX term is included in the statistical model; the estimated effect is often larger for the three models (2, 3, and 5) that include this square term, but some of the data subsets do not have sufficient degrees of freedom to allow the OXOX term to be estimated.

The results of these analyses are shown in Table 3, the Appendix Tables A1-1 to A1-3 and in Figures 1-1 to 1-3. Table 3 lists the Tech 4 studies together with a numerical code, the numbers of observations, vehicles, and fuels in each study, and the range of vehicle model years. The final row, with code 34, is for the entire Tech 4 subset. Tables A1-1 to A1-3 present the estimated value, lower bound (2.5^{th} percentile), and upper bound (97.5^{th} percentile), respectively, of the percentage change in NOx when oxygen changes from 2 to 3.5 % by weight. The same information is presented in Figures 1-1 to 1-3: The x-axis gives the numerical code of the data subset. The y-axis gives the estimated value and its confidence interval for each of the five statistical models 1-5. (Each line segment extends from the lower bound to the upper bound, and the estimated value is the marked value inside the confidence interval). Around each code value, the five models are shown in order; in several cases predictions are unavailable for one or more of these models. Note that the uncertainty of the predicted oxygen effect ranged from -100 % to +2.5E21 %; to make these plots readable, all values above 200 % were truncated at 200 %.

Table 3. Summary of Tech 4 Studies.						
Study	Code	Observations	Vehicles	Fuels	Minimum Year	Maximum Year
A/O-CURR	1	360	20	18	1989	1989
A/O-RVP/	2	224	20	12	1989	1989
A/O-SULF	3	20	10	2	1989	1989
A/O-TAME	4	20	10	2	1989	1989
AO-HVT90	5	270	10	27	1989	1989
AO-LOSLF	6	30	10	3	1989	1989
AO-SLFII	7	60	10	6	1989	1989
AOB17&18	8	256	22	13	1989	1995
APIAROM	9	90	10	9	1989	1990
APIRVPOX	10	48	8	6	1986	1989
ARBATLOX	11	70	7	10	1986	1991
ARBATLP2	12	19	5	4	1986	1990
ARBETOH	13	24	12	2	1990	1995
ARBMSD96	14	21	7	3	1986	1992
ARCO	15	50	10	5	1990	1990
ARCO5090	16	36	9	4	1990	1992
CHEVOX99	17	30	10	3	1988	1993
CHEVRON1	18	13	2	7	1987	1989
CHEVRON2	19	41	5	9	1987	1989
CHEVRON3	20	15	6	3	1986	1990
CHEVRON4	21	8	2	4	1989	1989
CHEVRON5	22	20	4	5	1989	1990
CHEVRON6	23	25	5	5	1987	1990
EPAEMFCT	24	1172	559	20	1986	1990
EPA_ATL1	25	243	38	8	1986	1990
EPA_ATL2	26	525	40	18	1986	1991
EPA_PH3	27	171	19	9	1986	1990
GMCONFRM	28	24	5	6	1989	1990
GMWSPA	29	30	5	6	1989	1990
NIPER-P1	30	20	4	5	1986	1986
NIPER-P2	31	40	4	10	1986	1986
UNOCAL	32	125	7	18	1988	1990
UNOCAL13	33	85	5	17	1988	1990
Tech 4	34	4185	900	203	1986	1995

Several aspects of the uncertainty can easily be seen in the Figures. For each subset code and model, the width of the confidence interval shows the wide uncertainty of the oxygen effect for individual studies and (for code 34), the lesser but still important uncertainty for Tech 4 as a whole. This confidence interval shows the uncertainty within a specific model and study. In many cases the confidence interval includes 0 %, showing that the oxygen change neither significantly increases nor significantly

decreases the NOx. The estimated percentage effect is sometimes positive and sometimes negative, and is sometimes significant (when the interval excludes zero). For a given study, the predictions of the five models are often very different, exhibiting the uncertainty due to the unknown model formulation. Furthermore, the wide variation between studies is apparent.

Since Tech 4 as a whole is a relatively large dataset, it is to be expected that the uncertainty intervals are much narrower for Tech 4 compared to the individual studies. The results show wide variation and inconsistency between the estimated effects for different studies and for the five different model formulations. Even for Tech 4 using Model 5 (ARB's model) the uncertainty (confidence interval) ranges from 4.0 to 7.5 %. Allowing for the additional uncertainty due to the five model formulations considered here expands this interval to the range 1.8 to 7.5 %. The interval is from 3.5 to 7.5 % for the models with the OXOX interaction.

The Tech 5 Model Ignores the Uncertainties Due to Variation Within and Between Studies and Across Model Formulations

Exactly the same analyses can be applied to the Tech 5 data as a whole and the individual Tech 5 studies. The results of these analyses are shown in Table 4, the Appendix Tables A2-1 to A2-3 and in Figure 2. Table 4 lists the Tech 5 studies together with a numerical code, the numbers of observations, vehicles, and fuels in each study, and the range of vehicle model years. The final row, with code 9, is for the entire Tech 5 subset. Tables A2-1 to A2-3 present the estimated value, lower bound (2.5^{th} percentile), and upper bound (97.5^{th} percentile), respectively, of the percentage change in NOx when oxygen changes from 2 to 3.5 % by weight. The same information is presented in Figure 2. Note that the predicted oxygen effects are unavailable for the AAMALOSU, CRCLOSUL, CRCLOSUO and CRC_E60 studies since oxygen was not varied in those studies. An important point is that we used exactly the same five model formulations as for the Tech 4 modeling, so that Model 5 is ARB's Tech 4 model formulation applied to the Tech 5 data rather than being ARB's Tech 5 offset model. Unlike the ARB's Tech 5 modeling approach, the linear and interaction terms are included for all Tech 5 studies, whether or not they were part of the experimental design for that study. The approach taken here takes into account the fact that the true response of a vehicle should not depend upon the experimental design. This approach also allows for a convenient comparison with the Tech 4 modeling results.

Table 4. Summary of Tech 5 Studies.						
Study	Code	Observations	Vehicles	Fuels	Minimum Year	Maximum Year
AAMALOSU	1	105	21	5	1997	1999
AAMSUOXY	2	65	13	6	.	.
CRCLOSUL	3	120	24	5	1997	1997
CRCLOSUO	4	48	24	2	1997	1997
CRC_E60	5	84	28	3	2000	2001
CRC_E67	6	326	12	12	2001	2003
EXXONMOBIL	7	20	5	4	1998	1999
TOYOTA	8	18	9	2	.	.
Tech 5	9	786	136	31	1997	2003

The Figures and Tables show the variation between and within the Tech 5 studies and between the five model formulations. The Tech 5 studies are generally more consistent than the Tech 4 studies. As expected, the uncertainty intervals are much narrower for Tech 5 compared to the individual studies. The results show wide variation and inconsistency between the different model formulations. Even for Tech 5 using Model 5 (ARB's Tech 4 model) the uncertainty (confidence interval) ranges from 1.3 to 9.2 %. Allowing for the additional uncertainty due to the five model formulations considered here expands this interval to the range 0.3 to 10.6 %. The interval is from 1.3 to 10.6 % for the models with the OXOX interaction.

The Tech 4 Model Ignores the Uncertainties Due to Variation In Response Between Vehicles Emitting Low and High NOx.

In this section we consider the dual model approach for Tech 4 that demonstrates how normal emitters and higher emitters respond differently to changes in fuel parameters.

As in previous modeling of normal and higher emitters, vehicles are defined as higher emitters if their "typical" emissions exceed a selected threshold of x g/mile. One possible choice for x is the Tech 4 NOx standard of 1 g/mile. In the EMFAC model, vehicles exceeding the NOx standard are designated as Moderate, High, Very High, or Super Emitters, and vehicles not exceeding the NOx standard are designated as Normal Emitters. Previous modeling results suggested that the best fitting dual models used a cutoff of approximately 0.4 to 0.6 g/mile, so we also evaluated defining higher and normal emitters using the cutoffs of 0.4 and 0.6 g/mile. These two cutoffs are not used in the EMFAC model so the current EMFAC model would need to be specially adapted to allow for these alternative cutoffs to be used with the Predictive Model. Previously the "typical" emissions for a vehicle was defined as the average vehicle emissions, calculated by first averaging the NOx emissions across each fuel, and then averaging over the fuels tested on that vehicle. Some have criticized this approach as causing the higher emitter group to be biased toward vehicles tested on higher-emitting fuels, although this bias is likely to be small because the variation between vehicles is generally much large than variation between fuels on the same vehicle. Nevertheless, for this modeling exercise we defined the "typical" vehicle emissions as the average

over the Auto/Oil study Fuel A, since this was the base fuel for the Auto/Oil studies that form a large fraction of the Tech 4 database.

For most of the Auto/Oil studies and for two other Tech 4 studies, one of the test fuels was Auto/Oil fuel A or had exactly the same fuel parameters as fuel A. In those cases, the NOx emissions level for a vehicle is calculated as the average of the emissions tests on fuel A or its equivalent. (This is the same as the emissions on fuel A, since the Tech 4 data have already been averaged across each vehicle/fuel combination). In other cases, instead of using fuel A we used the vehicle's NOx emissions on the "closest" fuel to fuel A, where the distance between fuel A and another fuel B is defined in a Euclidean manner as

$$\text{Distance} = \Sigma \{P(A) - P(B)\} \{P(A) - P(B)\} / \text{Var}(P),$$

where P(A) is the value of a fuel parameter on fuel A, P(B) is the value of the same fuel parameter on fuel B, Var(P) is the variance of the fuel parameter across all observations in the Tech group, and the sum is over the seven fuel parameters. These calculations use the raw fuel parameter values rather than the values renormalized to have a mean of zero and a variance of 1. Using this distance metric, differences between parameters like sulfur that varied significantly over the database were downweighted by the variance so they would not dominate the metric. By definition, the distance between fuel A and itself is zero, but for some vehicles all the distances were non-zero since the vehicle was not tested on a fuel with the same parameters as fuel A.

Using this distance metric and the three cutoffs (100 %, 60 % and 40 % of the NOx standard), three alternative higher and normal emitter definitions were evaluated. For each vehicle, let Min denote the minimum distance between fuel A and all the fuels tested. The emissions level for that vehicle is defined as the average emissions on the fuel closest to fuel A. This emissions level is compared with the cutoff (as a percentage of 1 g/mile NOx) to decide if the vehicle is a normal or higher emitter.

- d = 0, cutoff = 100 %: Only use vehicles where Min = 0. This excludes vehicles not tested on fuel A.
- d = 0, cutoff = 60 %: Only use vehicles where Min = 0. This excludes vehicles not tested on fuel A.
- d = 0, cutoff = 40 %: Only use vehicles where Min = 0. This excludes vehicles not tested on fuel A.
- d = 5, cutoff = 100 %: Only use vehicles where Min <= 5. This includes some vehicles not tested on fuel A.
- d = 5, cutoff = 60 %: Only use vehicles where Min <= 5. This includes some vehicles not tested on fuel A.
- d = 5, cutoff = 40 %: Only use vehicles where Min <= 5. This includes some vehicles not tested on fuel A.
- d = 25, cutoff = 100 %: Only use vehicles where Min <= 25. All vehicles are included.
- d = 25, cutoff = 60 %: Only use vehicles where Min <= 25. All vehicles are included.
- d = 25, cutoff = 40 %: Only use vehicles where Min <= 25. All vehicles are included.

For d = 0, only 86 vehicles were tested on fuel A. The remaining 814 vehicles were not used for these dual models. Therefore the results with d= 0 are not expected to be very precise. For d = 5, only 248 vehicles were tested on a fuel within distance 5 from fuel A. The remaining 652 vehicles were not used for this dual model. For d= 25, all vehicles are included in the dual model since the maximum distance from fuel A among all Tech 4 vehicles was 22.0.

We computed the confidence intervals for each of the normal and higher emitter subsets as well as for Tech 4 as a whole. The results of these analyses are shown in Table 5, the Appendix Tables A3-1 to A3-3 and in Figures 3-1 to 3-2. Table 5 lists the normal and higher emitter subsets together with a numerical code, the numbers of observations, vehicles, and fuels in each subset, and the range of vehicle model years. The final row, with code 19, is for the entire Tech 4 subset. Tables A3-1 to A3-3 present the estimated value, lower bound (2.5^{th} percentile), and upper bound (97.5^{th} percentile), respectively, of the percentage change in NOx when oxygen changes from 2 to 3.5 % by weight. The same information is presented in Figures 3-1 to 3-2. The normal and higher emitter subsets are arranged so that each normal emitter subset is followed by the corresponding higher emitter subset.

Table 5. Summary of Tech 4 Normal and Higher Emitter Subsets.						
Study	Code	Observations	Vehicles	Fuels	Minimum Year	Maximum Year
Normal, d=0, cutoff=100	1	1142	81	93	1988	1994
Higher, d=0, cutoff=100	2	89	5	58	1989	1989
Normal, d=0, cutoff=60	3	594	44	93	1988	1994
Higher, d=0, cutoff=60	4	637	42	87	1989	1994
Normal, d=0, cutoff=40	5	368	26	93	1988	1994
Higher, d=0, cutoff=40	6	863	60	92	1988	1994
Normal, d=5, cutoff=100	7	2161	210	136	1986	1994
Higher, d=5, cutoff=100	8	455	38	76	1986	1990
Normal, d=5, cutoff=60	9	1368	145	136	1986	1994
Higher, d=5, cutoff=60	10	1248	103	114	1986	1994
Normal, d=5, cutoff=40	11	791	81	132	1986	1994
Higher, d=5, cutoff=40	12	1825	167	130	1986	1994
Normal, d=25, cutoff=100	13	3535	779	203	1986	1995
Higher, d=25, cutoff=100	14	650	121	100	1986	1990
Normal, d=25, cutoff=60	15	2359	537	203	1986	1995
Higher, d=25, cutoff=60	16	1826	363	152	1986	1994
Normal, d=25, cutoff=40	17	1323	274	194	1986	1995
Higher, d=25, cutoff=40	18	2862	626	189	1986	1994
Tech 4	19	4185	900	203	1986	1995

For these analyses, the most important results are the comparisons between the normal and higher emitter subsets that use the same definitions for d and the cutoff percentage. In every case with d = 5 or d = 25, the percentage change in NOx for an oxygen increase from 2 to 3.5 % was greater for the normal emitters compared to the higher emitters. The same was true for slightly more than half of the cases where d = 0 (For some reason this always held for the 100 % cutoff but never held for the 60 % cutoff).

It is also useful to compare the weighted average predictions of the single and dual models. For the cutoffs of 60 % or 40 % of the standard, emissions weights are not currently available from the EMFAC model. For the cutoff of 1 g/mile, emissions weights for 2010 using the latest version of EMFAC are also not available, but we can use the emissions weights for 2005 shown in Table 2, which were based on EMFAC 2005, as an approximation. The year 2005 weights are likely to be conservative in the sense of underestimating the emissions contribution of higher emitters in 2010, due to the tendency for emissions to increase with age.

Table 6 shows the 95 % confidence intervals for the fleet-weighted average percentage changes in NOx when oxygen changes from 2 to 3.5 % by weight. For this calculation, the estimated changes in the logarithm of NOx for normal and higher emitters were weighted using the emissions weights. Also shown, for comparison, are the confidence intervals for Tech 4, the “single” model. Figure 4 is a plot of the same data. Using the 1 g/mile cutoff and d >= 5 (since the strict criterion d=0 results in a small database with large uncertainty), the weighted average percentage change in NOx ranges from -3.92 to 9.20 %.

Table 6. 95 % Confidence Intervals for Fleet Average Emissions Effects Using Dual and Single Models with 100 % Cutoff.

D	Value	M1	M2	M3	M4	M5
0	Estimate	0.05	-7.32	1.69	-3.60	3.79
0	Lower Bound	-2.85	-15.40	-10.46	-16.61	-11.79
0	Upper Bound	3.03	1.53	15.49	11.43	22.11
5	Estimate	0.44	-0.30	4.61	4.11	4.06
5	Lower Bound	-0.87	-3.92	1.26	-0.75	-0.73
5	Upper Bound	1.78	3.46	8.06	9.20	9.09
25	Estimate	1.31	1.20	2.28	1.35	1.59
25	Lower Bound	0.38	-1.02	1.10	-0.87	-0.64
25	Upper Bound	2.26	3.47	3.46	3.61	3.86
Single	Estimate	2.44	5.22	3.67	5.59	5.71
Single	Lower Bound	1.75	3.49	2.84	3.85	3.96
Single	Upper Bound	3.14	6.98	4.50	7.36	7.49

For each choice of d and the cutoff, we also tested whether the dual model fitted the data significantly better. For these model comparisons we used the ML method instead of REML. In every case we were able to fit all six linear terms in Models 1-4, so the single model with the same set of model terms is a special case of the more general dual model with the same terms for the normal and higher emitter subsets. Thus the likelihood ratio test defined by twice the difference in log-likelihoods can be applied

(assuming the samples are sufficiently large). We first compared the dual models to the corresponding single models fitted to the combined normal and higher emitter data (for d = 0 and d = 5, this combined dataset is much smaller than the Tech 4 database). This comparison allows for differences in either the vehicle intercepts or the fuel effects or both. All the p-values were significant at levels below 10^{-10} except for the cases where d = 0 where the p-values were at most 0.008. We then compared the dual models to the same single model except that instead of having an overall intercept for the fixed and random effects, separate fixed and random intercept terms were fitted to the normal and higher emitters. This second comparison allows for differences in only the fuel effects. All the p-values were significant at levels below 10^{-10} except for the cases where d = 0 where the p-values were at most 0.01 for the cutoffs of 40 % and 60 % and were not significant for the 100 % cutoff. The lack of significance for the d=0, 100 % cutoff case is likely due to the very small number of higher emitter observations (89) for this case. These results demonstrate that the dual models fit statistically significantly better than the single models and the fuel responses are statistically significantly different.

Finally, we used the log-likelihoods to compare the dual models using different cutoffs. For each model, the 60 % cutoff gave the best-fitting dual model (highest log-likelihood), the 40 % cutoff was second best, and the 100 % cutoff gave the poorest fit among these three alternatives. However, the statistical analyses does not show that the 60 % cutpoint is statistically significantly better than the other cutpoints since these log-likelihood comparisons are not a valid statistical hypothesis test. Instead the most important result is that the analysis shows the general pattern that the highest emitters respond differently to the lowest emitters, and that the lowest emitters have the highest NOx response to oxygen.

Some reviewers of this approach have tried to suggest that the higher/normal emitter analysis is not justified without some sort of engineering justification for the best-fitting cutpoint. Our main response is that our analysis suggests that in reality we believe that the NOx response to oxygen and other fuel changes varies continuously with the emissions level rather than suddenly changing from one function to another at the selected higher emitter cutoff. Instead of attempting to fit and use a much more complex emissions model where the coefficients are some function of the emissions level, we instead use a reasonable and much simpler approximation that has only two response functions, keeping the general pattern that the highest emitters respond differently to the lowest emitters. There is also a possible “engineering” explanation that the change in response to oxygen might be due to the effect of catalyst aging, so that emissions from fresher catalysts are not as stable. This might be part of the reason for the much narrower uncertainty ranges for the Tech 5 studies which tended to use “aged catalysts.” Of course there are also technology differences that might also be part of the explanation of the lower variability in Tech 5.

Other reviewers of this approach have asked for studies that specifically looked for and found different responses for higher NOx emitters. There were two studies that examined high emitters, namely the Auto/Oil High emitter study (excluded from the Predictive Model database) and the EPA/ATL-Phase I and II Reformulated Gasoline / Oxygenated Blend Study (included in the database). The EPA/ATL study reported different fuel responses by the High emitter vehicles. However, these studies defined the High emitters based on the THC and CO emissions rather than directly by the NOx

emissions (although high THC and CO emitters tend to be low NOx emitters). Unfortunately, we are not aware of any studies that were designed to look into the fuel effects on High NOx emitters but we would certainly welcome such studies to be performed. In our view the absence of a study that was originally designed to look at fuel effects on higher NOx emitters does not mean that the effect that we found in our meta-analysis of the Predictive Model database does not exist.

Summary

The main points can be summarized in the following bullets.

- The Predictive Model database is not a random sample from the California on-road fleet but is instead a database compiled from several emissions studies.
- The Predictive Model database is not representative of the California on-road fleet since the model year and NOx emissions distributions are unrepresentative.
- The Predictive Model database is unrepresentative of current California gasolines because many of the test fuels do not meet current California standards, especially with respect to sulfur. This introduces an extra uncertainty due to the need to extrapolate fuel effects on those vehicles from the more extreme fuels.
- The current and proposed ARB Predictive Models ignore uncertainties in the database, coefficients, and model formulation when determining compliance.
- Estimates of NOx changes due to oxygen for individual Tech 4 and Tech 5 studies tend to vary in direction and statistical significance.
- Most estimates of NOx changes due to oxygen for individual Tech 4 and Tech 5 studies have large uncertainties.
- Estimates of NOx changes vary between different model formulations.
- The current Tech 4 model gives an estimated NOx percentage change of 5.7 % due to oxygen changing from 2 to 3.5 %. Because of sampling uncertainty about the model coefficients, the confidence interval ranges from 4.0 to 7.5 %.
- Different models for Tech 4 as a whole give estimated NOX percentage changes ranging from 1.8 to 7.5 % due to oxygen changing from 2 to 3.5 %.
- Different models for Tech 5 as a whole give estimated NOX percentage changes ranging from 0.3 to 10.6 % due to oxygen changing from 2 to 3.5 %.
- Dual models that assume different fuel responses for higher-emitting vehicles fit the data statistically significantly better. The best fitting of the three cutpoints tested was consistently at cutpoint 60 %.
- Dual models that assume different fuel responses for higher-emitting vehicles show in most cases that higher emitters show a lower response to oxygen than normal emitters.
- Catalyst aging might provide a possible engineering explanation for this phenomenon.
- Using the 1 g/mile cutoff and d >= 5 gives an estimated NOx percentage change ranging from -3.9 to 9.2 % due to oxygen changing from 2 to 3.5 %.

Putting all these points together it is clear that the estimated effects of oxygen (or other fuel parameter) changes on NOx are quite uncertain and that the uncertainty of the current ARB estimates is comparable with the uncertainty of the estimates from the dual model approach. Despite these uncertainties with the database and the statistical

model, the current ARB approach bases the Predictive Model regulations on the estimated fixed effects from their preferred model, not even taking into account the fact that even if their fitted statistical model was exactly correct, those model predictions have substantial uncertainty due to the random effect and residual error terms. We recommend that the ARB take into account the uncertainty in their model predictions.

There are several ways that the ARB could account for uncertainty in their model predictions. Here are some alternatives. One reasonable and highly flexible approach would be for the ARB to define several feasible statistical models, including the dual models described here, and define compliance using the lowest lower confidence bound amongst those statistical models. In that manner, a fuel would be judged non-compliant only if there was a statistically significant NOx increase at the 2.5 % level for every feasible model (the confidence levels in these analyses could easily be changed to be 90 % in order to make this one-sided significance level the more usual 5 %). A second approach would use the highest lower confidence bound, so that a fuel is non-compliant if there was a statistically significant increase for one or more feasible model. A third approach would define compliance based on the lowest prediction from all feasible models (this accounts for the uncertainty about the statistical model but not the uncertainty within the given model). A fourth approach would define compliance based on the lower confidence bound from the model selected to be the best-fitting (this accounts for the uncertainty within the statistical model but not the uncertainty about the given model). For example, for Tech 4, a feasible set of models might be chosen as the single models M2, M3 and M5 with OX and OXOX terms, and the dual models M2, M3, and M5 with d >= 5, and cutoff 100 %.[4] The lowest lower confidence bound for the NOx change due to oxygen changing from 2 to 3.5 % equals -3.9 %. The highest lower confidence bound equals 4.0 %. The lowest predicted value equals -0.3 %. The lower confidence interval from the dual model M5 with d=25 equals -0.6 %. For this example the fuel with 3.5 % oxygen and all other parameters at their base values would be NOx compliant using the first, third and fourth approaches but not the second approach. These calculations could be easily implemented using the random balance method.[5]

[4] Including the single models as feasible is a conservative approach in view of the fact that the dual models fit the data statistically significantly better.

[5] Randomly select a set of fuels uniformly within suitable parameter ranges for all seven fuel parameters. For each randomly selected fuel, use SAS software to calculate the compliance value (e.g. lowest lower confidence bound). Fit a multiple linear regression model to these fuels to estimate the compliance value as a linear combination of the fuel parameters and interactions. The coefficients of this multiple linear regression model are entered into the Predictive Model Excel spreadsheet.

Fig 1-1. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Studies

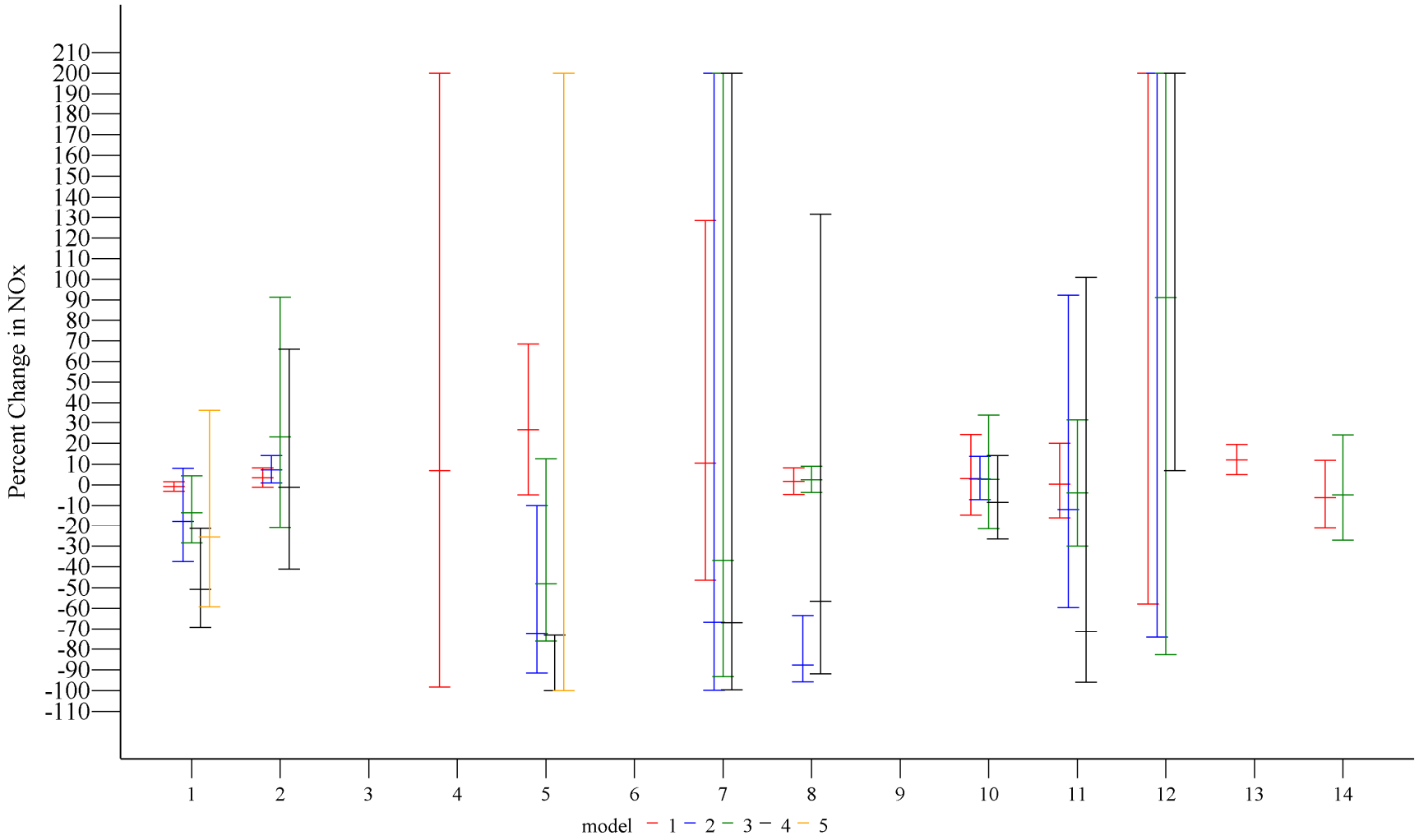


Fig 1-2. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Studies

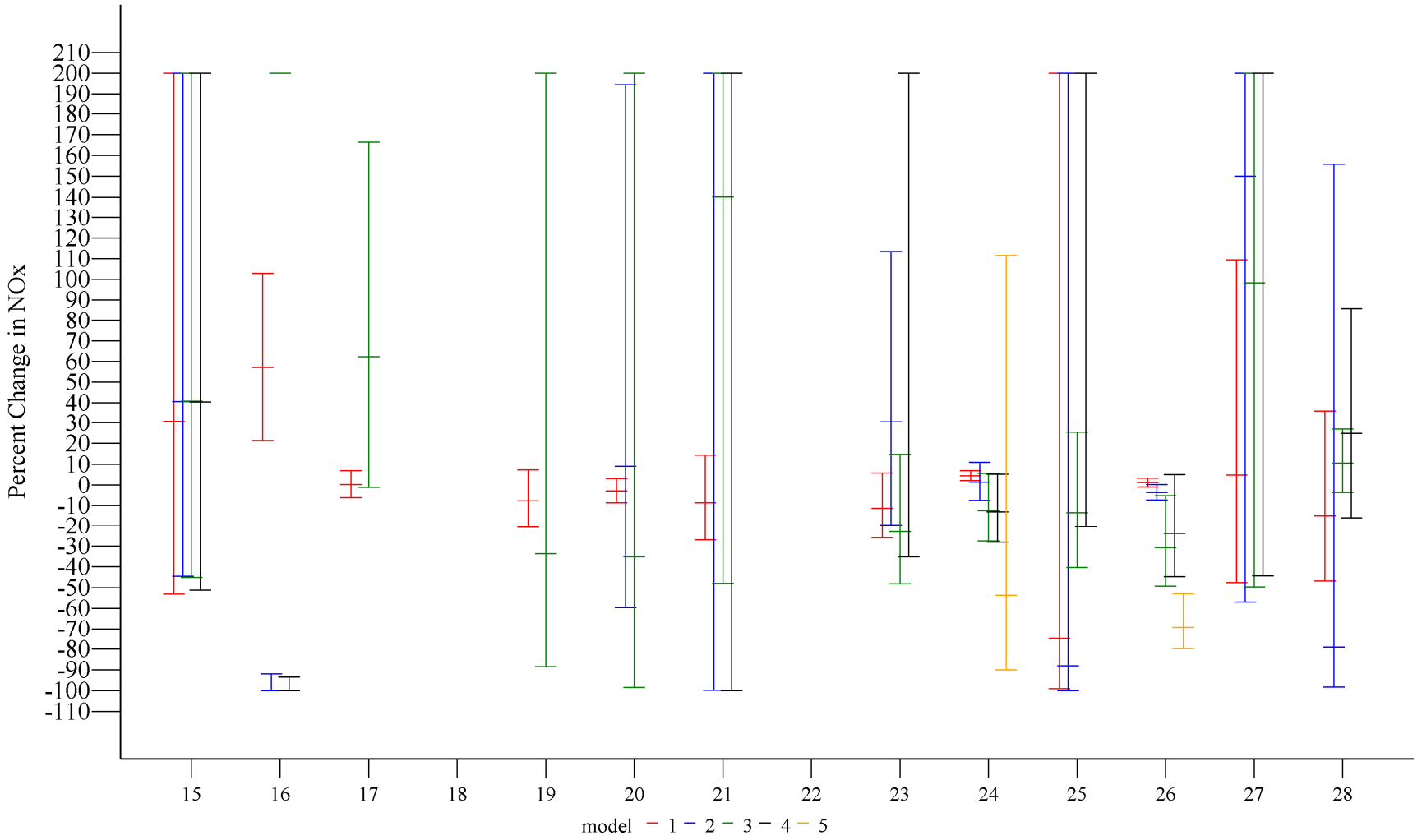


Fig 1-3. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Studies

Subsets 29 to 34

Estimated Percent Change and a 95 % Confidence Interval

Percentages Above 200 % Are Truncated to 200 for Plotting

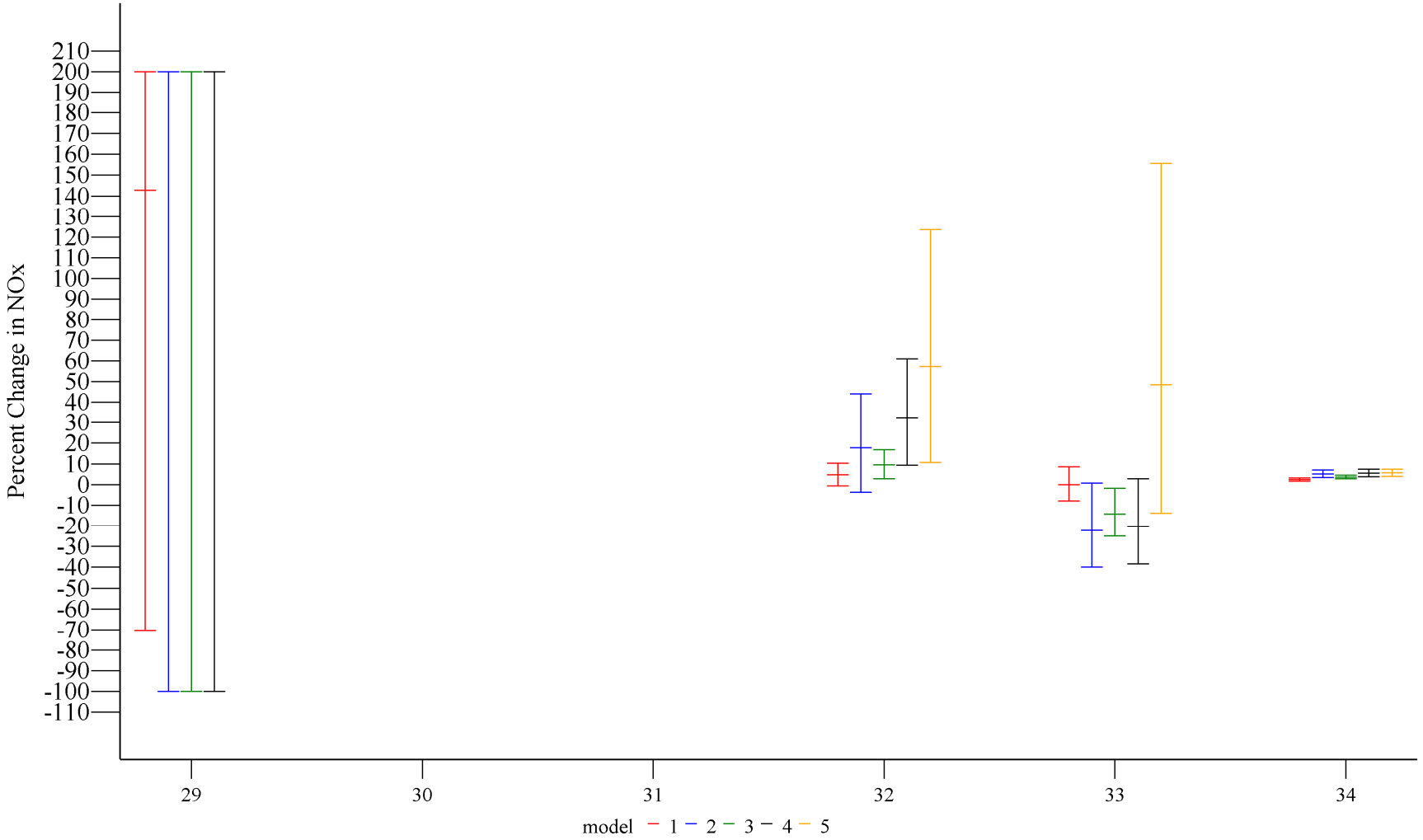


Fig 2. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 5 Studies

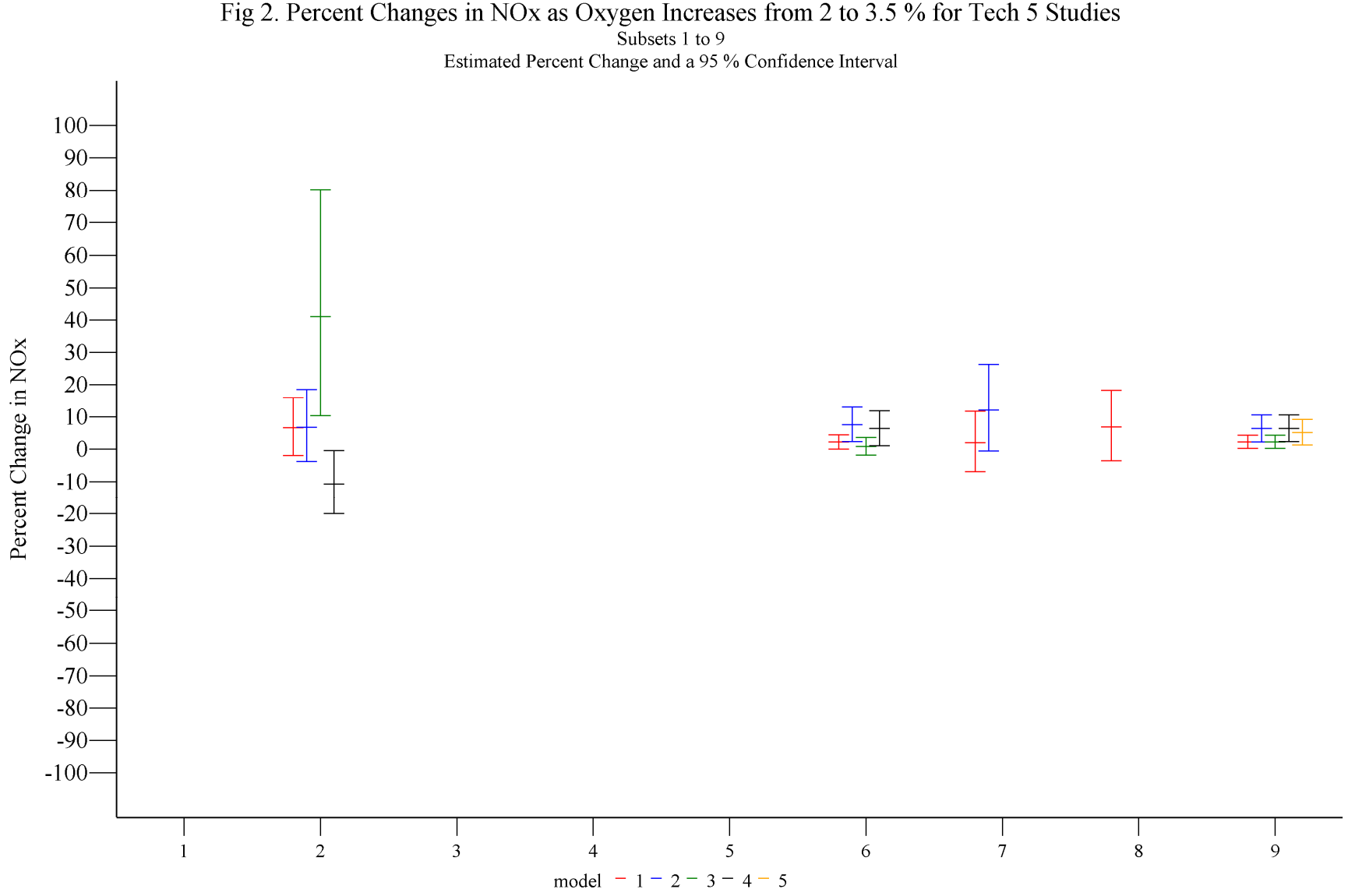


Fig 3-1. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Normal and Higher Emitters

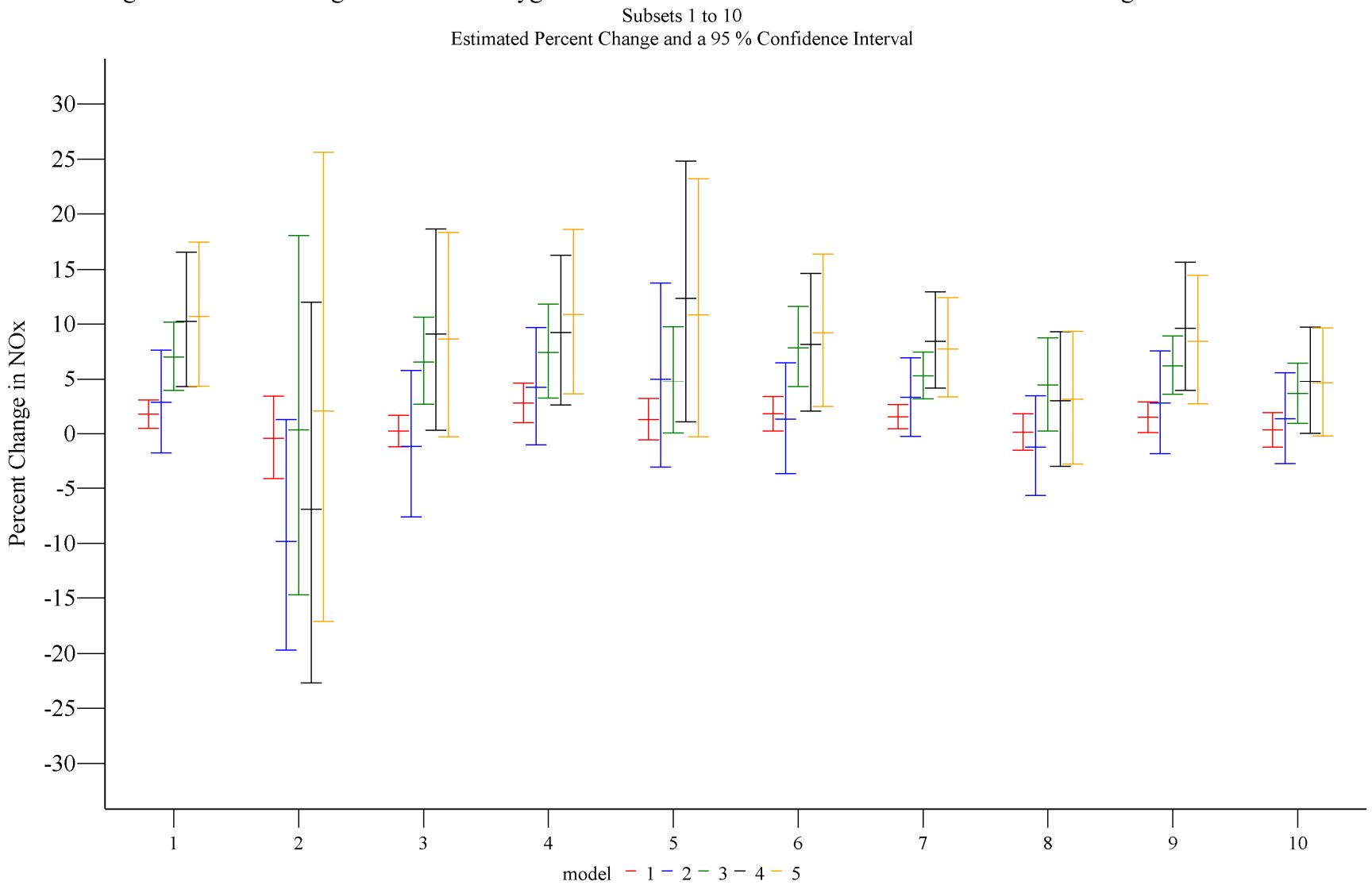


Fig 3-2. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Normal and Higher Emitters

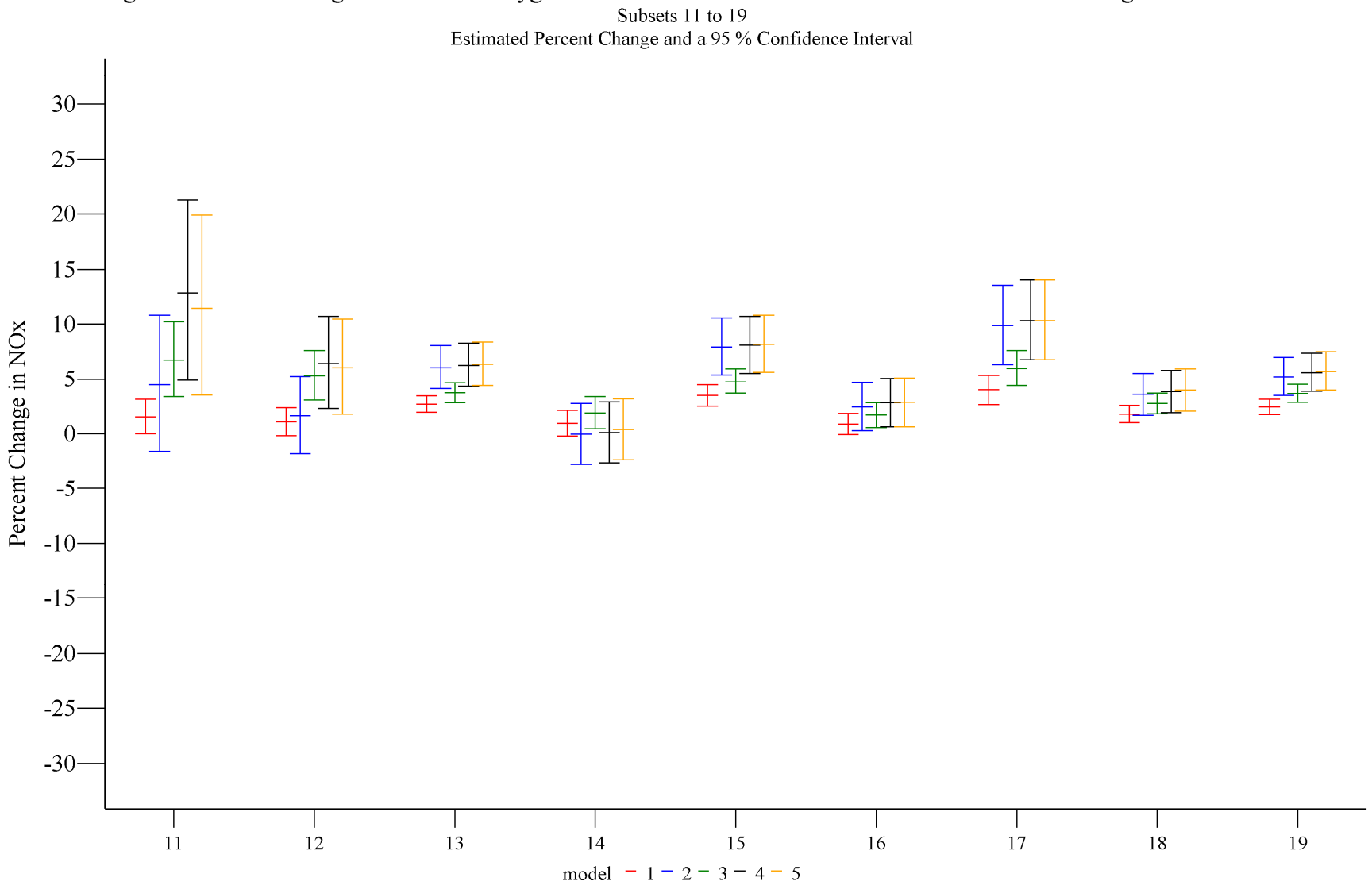
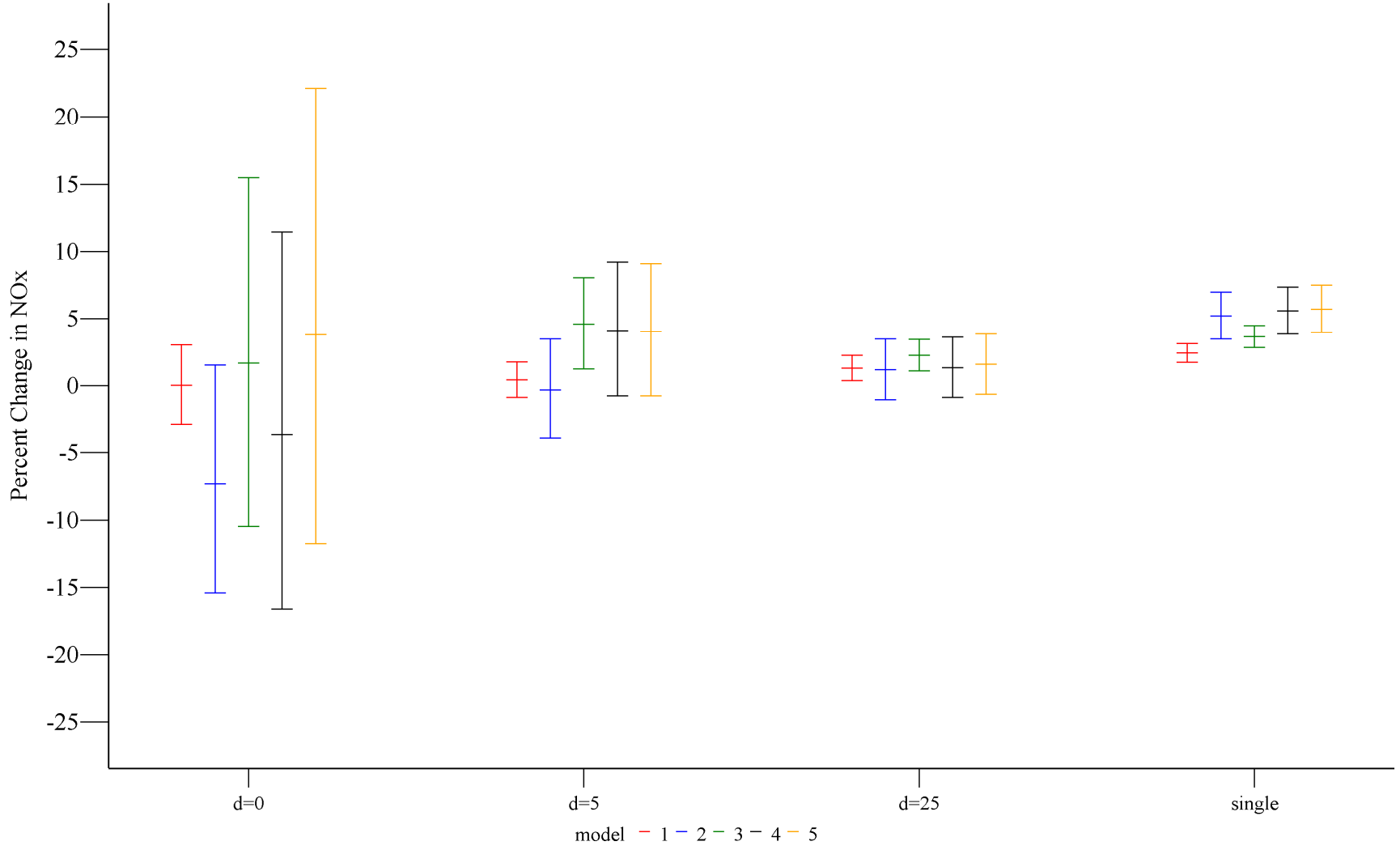


Fig 4. Weighted Averages for Dual and Single Models for 2005 based on EMFAC 2000

Dual Model Cutoff = 1 g/mile

Estimated Percent Change and a 95 % Confidence Interval



APPENDIX

Table A1-1. Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 4 Studies.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
A/O-CURR	1	-0.80	-17.74	-13.50	-50.87	-25.53
A/O-RVP/	2	3.44	7.30	23.07	-1.13	.
A/O-SULF	3	.	.	.	.	.
A/O-TAME	4	6.82	.	.	.	.
AO-HVT90	5	26.57	-72.44	-48.18	-99.85	-99.96
AO-LOSLF	6	.	.	.	.	.
AO-SLFII	7	10.57	-66.77	-36.86	-66.91	.
AOB17&18	8	1.61	-87.59	2.49	-56.61	.
APIAROM	9	.	.	.	.	.
APIRVPOX	10	3.06	2.79	2.62	-8.41	.
ARBATLOX	11	0.43	-11.92	-3.88	-71.49	.
ARBATLP2	12	932.12	1221.01	91.16	3589.57	.
ARBETOH	13	12.00	.	.	.	.
ARBMSD96	14	-6.11	.	-4.93	.	.
ARCO	15	30.63	40.60	40.72	40.43	.
ARCO5090	16	57.01	-99.76	4081.24	-99.85	.
CHEVOX99	17	0.19	.	62.28	.	.
CHEVRON1	18	.	.	.	.	.
CHEVRON2	19	-7.70	.	-33.66	.	.
CHEVRON3	20	-3.00	9.06	-35.21	.	.
CHEVRON4	21	-8.62	5383.89	140.17	2902.09	.
CHEVRON5	22	.	.	.	.	.
CHEVRON6	23	-11.41	30.96	-22.84	262.08	.
EPAEMFCT	24	4.44	1.29	-12.56	-13.00	-53.76
EPA_ATL1	25	-74.82	-88.11	-13.44	201.42	.
EPA_ATL2	26	1.10	-3.65	-30.76	-23.78	-69.27
EPA_PH3	27	4.80	150.12	98.28	204.48	.
GMCONFRM	28	-15.02	-78.95	10.54	24.93	.
GMWSPA	29	142.77	1.13E+08	8.09E+06	3.17E+07	.
NIPER-P1	30	.	.	.	.	.
NIPER-P2	31	.	.	.	.	.
UNOCAL	32	4.70	17.78	9.56	32.60	57.35
UNOCAL13	33	0.05	-22.27	-14.14	-20.41	48.50
Tech 4	34	2.44	5.22	3.67	5.59	5.71

Table A1-2. Lower Confidence Bounds for Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 4 Studies.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
A/O-CURR	1	-3.10	-37.39	-28.36	-69.29	-59.32
A/O-RVP/	2	-1.17	0.82	-20.85	-41.07	.
A/O-SULF	3	.	.	.	.	.
A/O-TAME	4	-98.31	.	.	.	.
AO-HVT90	5	-4.91	-91.57	-76.17	-100.00	-100.00
AO-LOSLF	6	.	.	.	.	.
AO-SLFII	7	-46.47	-99.84	-93.28	-99.54	.
AOB17&18	8	-4.60	-95.77	-3.60	-91.87	.
APIAROM	9	.	.	.	.	.
APIRVPOX	10	-14.58	-7.09	-21.45	-26.47	.
ARBATLOX	11	-15.96	-59.65	-29.90	-95.96	.
ARBATLP2	12	-57.98	-74.32	-82.71	6.78	.
ARBETOH	13	4.99	.	.	.	.
ARBMSD96	14	-21.15	.	-27.14	.	.
ARCO	15	-53.10	-44.44	-45.10	-51.17	.
ARCO5090	16	21.49	-99.99	440.73	-100.00	.
CHEVOX99	17	-6.13	.	-1.15	.	.
CHEVRON1	18	.	.	.	.	.
CHEVRON2	19	-20.60	.	-88.50	.	.
CHEVRON3	20	-8.74	-59.59	-98.39	.	.
CHEVRON4	21	-26.95	-99.84	-47.95	-99.93	.
CHEVRON5	22	.	.	.	.	.
CHEVRON6	23	-25.74	-19.64	-48.14	-35.23	.
EPAEMFCT	24	2.15	-7.43	-27.51	-27.98	-89.89
EPA_ATL1	25	-99.05	-99.98	-40.23	-20.33	.
EPA_ATL2	26	-1.05	-7.35	-49.40	-44.68	-79.89
EPA_PH3	27	-47.56	-56.93	-49.75	-44.31	.
GMCONFRM	28	-46.87	-98.27	-3.75	-15.99	.
GMWSPA	29	-70.29	-100.00	-100.00	-100.00	.
NIPER-P1	30	.	.	.	.	.
NIPER-P2	31	.	.	.	.	.
UNOCAL	32	-0.55	-3.73	2.79	9.30	10.72
UNOCAL13	33	-7.87	-40.02	-25.02	-38.43	-13.77
Tech 4	34	1.75	3.49	2.84	3.85	3.96

Table A1-3. Upper Confidence Bounds for Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 4 Studies.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
A/O-CURR	1	1.55	8.08	4.45	-21.38	36.32
A/O-RVP/	2	8.26	14.19	91.36	65.86	.
A/O-SULF	3	.	.	.	.	.
A/O-TAME	4	6635.43	.	.	.	.
AO-HVT90	5	68.48	-9.95	12.68	-73.29	28137.29
AO-LOSLF	6	.	.	.	.	.
AO-SLFII	7	128.37	6803.01	492.94	2264.15	.
AOB17&18	8	8.23	-63.59	8.96	131.49	.
APIAROM	9	.	.	.	.	.
APIRVPOX	10	24.34	13.73	34.06	14.10	.
ARBATLOX	11	20.01	92.31	31.80	101.06	.
ARBATLP2	12	25254.28	67862.25	2013.74	1.27E+05	.
ARBETOH	13	19.48	.	.	.	.
ARBMSD96	14	11.79	.	24.04	.	.
ARCO	15	263.84	255.81	260.70	303.82	.
ARCO5090	16	102.91	-91.92	32231.62	-93.50	.
CHEVOX99	17	6.94	.	166.40	.	.
CHEVRON1	18	.	.	.	.	.
CHEVRON2	19	7.30	.	282.54	.	.
CHEVRON3	20	3.11	194.36	2501.27	.	.
CHEVRON4	21	14.31	1.85E+08	1008.08	1.35E+08	.
CHEVRON5	22	.	.	.	.	.
CHEVRON6	23	5.69	113.42	14.81	1923.98	.
EPAEMFCT	24	6.79	10.83	5.48	5.09	111.56
EPA_ATL1	25	570.49	9065.47	25.37	1040.39	.
EPA_ATL2	26	3.30	0.20	-5.24	5.02	-53.03
EPA_PH3	27	109.43	1352.52	682.44	1564.57	.
GMCONFRM	28	35.91	155.75	26.95	85.77	.
GMWSPA	29	1883.50	2.52E+21	5.53E+17	5.61E+19	.
NIPER-P1	30	.	.	.	.	.
NIPER-P2	31	.	.	.	.	.
UNOCAL	32	10.21	44.09	16.79	60.86	123.63
UNOCAL13	33	8.64	0.74	-1.69	2.89	155.74
Tech 4	34	3.14	6.98	4.50	7.36	7.49

Table A2-1. Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 5 Studies.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
AAMALOSU	1	.	.	.	.	.
AAMSUOXY	2	6.63	6.76	41.01	-10.74	.
CRCLOSUL	3	.	.	.	.	.
CRCLOSUO	4	.	.	.	.	.
CRC_E60	5	.	.	.	.	.
CRC_E67	6	2.21	7.53	0.83	6.36	.
EXXONMOBIL	7	1.96	12.04	.	.	.
TOYOTA	8	6.83	.	.	.	.
Tech 5	9	2.28	6.36	2.27	6.36	5.17

Table A2-2. Lower Confidence Bounds for Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 5 Studies.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
AAMALOSU	1	.	.	.	.	.
AAMSUOXY	2	-1.90	-3.82	10.30	-19.95	.
CRCLOSUL	3	.	.	.	.	.
CRCLOSUO	4	.	.	.	.	.
CRC_E60	5	.	.	.	.	.
CRC_E67	6	0.00	2.31	-1.84	1.10	.
EXXONMOBIL	7	-6.96	-0.59	.	.	.
TOYOTA	8	-3.52	.	.	.	.
Tech 5	9	0.30	2.28	0.30	2.29	1.29

Table A2-3. Upper Confidence Bounds for Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 5 Studies.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
AAMALOSU	1	.	.	.	.	.
AAMSUOXY	2	15.89	18.51	80.27	-0.47	.
CRCLOSUL	3	.	.	.	.	.
CRCLOSUO	4	.	.	.	.	.
CRC_E60	5	.	.	.	.	.
CRC_E67	6	4.47	13.00	3.58	11.88	.
EXXONMOBIL	7	11.73	26.27	.	.	.
TOYOTA	8	18.29	.	.	.	.
Tech 5	9	4.29	10.60	4.29	10.60	9.20

Table A3-1. Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 4 Normal and Higher Emitters.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
Normal, d=0, cutoff=100	1	1.77	2.85	7.01	10.25	10.71
Higher, d=0, cutoff=100	2	-0.40	-9.80	0.35	-6.91	2.06
Normal, d=0, cutoff=60	3	0.25	-1.12	6.58	9.10	8.64
Higher, d=0, cutoff=60	4	2.78	4.21	7.43	9.24	10.87
Normal, d=0, cutoff=40	5	1.30	5.02	4.79	12.32	10.83
Higher, d=0, cutoff=40	6	1.81	1.31	7.87	8.16	9.20
Normal, d=5, cutoff=100	7	1.55	3.29	5.31	8.45	7.76
Higher, d=5, cutoff=100	8	0.16	-1.21	4.43	3.00	3.12
Normal, d=5, cutoff=60	9	1.50	2.78	6.23	9.63	8.44
Higher, d=5, cutoff=60	10	0.35	1.37	3.66	4.77	4.61
Normal, d=5, cutoff=40	11	1.55	4.43	6.74	12.81	11.41
Higher, d=5, cutoff=40	12	1.09	1.65	5.31	6.42	6.03
Normal, d=25, cutoff=100	13	2.69	6.06	3.73	6.27	6.36
Higher, d=25, cutoff=100	14	0.95	-0.03	1.90	0.10	0.38
Normal, d=25, cutoff=60	15	3.47	7.94	4.81	8.08	8.17
Higher, d=25, cutoff=60	16	0.89	2.44	1.70	2.82	2.86
Normal, d=25, cutoff=40	17	3.99	9.86	5.98	10.33	10.33
Higher, d=25, cutoff=40	18	1.79	3.58	2.74	3.84	3.98
Tech 4	19	2.44	5.22	3.67	5.59	5.71

Table A3-2. Lower Confidence Bounds for Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 4 Normal and Higher Emitters.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
Normal, d=0, cutoff=100	1	0.49	-1.74	3.94	4.27	4.32
Higher, d=0, cutoff=100	2	-4.06	-19.68	-14.72	-22.63	-17.09
Normal, d=0, cutoff=60	3	-1.16	-7.59	2.67	0.32	-0.26
Higher, d=0, cutoff=60	4	1.01	-1.01	3.23	2.60	3.64
Normal, d=0, cutoff=40	5	-0.55	-3.02	0.06	1.07	-0.27
Higher, d=0, cutoff=40	6	0.26	-3.61	4.26	2.04	2.46
Normal, d=5, cutoff=100	7	0.46	-0.25	3.18	4.14	3.33
Higher, d=5, cutoff=100	8	-1.47	-5.64	0.26	-2.94	-2.75
Normal, d=5, cutoff=60	9	0.11	-1.78	3.60	3.92	2.71
Higher, d=5, cutoff=60	10	-1.20	-2.69	0.94	0.05	-0.21
Normal, d=5, cutoff=40	11	0.00	-1.58	3.38	4.95	3.52
Higher, d=5, cutoff=40	12	-0.18	-1.81	3.05	2.31	1.77
Normal, d=25, cutoff=100	13	1.94	4.11	2.83	4.31	4.39
Higher, d=25, cutoff=100	14	-0.21	-2.76	0.45	-2.62	-2.35
Normal, d=25, cutoff=60	15	2.50	5.39	3.68	5.54	5.62
Higher, d=25, cutoff=60	16	-0.05	0.28	0.57	0.62	0.65
Normal, d=25, cutoff=40	17	2.65	6.32	4.39	6.78	6.78
Higher, d=25, cutoff=40	18	1.00	1.66	1.82	1.92	2.04
Tech 4	19	1.75	3.49	2.84	3.85	3.96

Table A3-3. Upper Confidence Bounds for Percentage Changes in NOx as Oxygen Changes from 2 to 3.5 % for Tech 4 Normal and Higher Emitters.						
Study	Code	Model 1	Model 2	Model 3	Model 4	Model 5
Normal, d=0, cutoff=100	1	3.08	7.65	10.18	16.57	17.49
Higher, d=0, cutoff=100	2	3.41	1.30	18.07	12.00	25.63
Normal, d=0, cutoff=60	3	1.69	5.80	10.64	18.65	18.33
Higher, d=0, cutoff=60	4	4.59	9.70	11.81	16.30	18.61
Normal, d=0, cutoff=40	5	3.19	13.73	9.75	24.83	23.17
Higher, d=0, cutoff=40	6	3.37	6.49	11.59	14.65	16.38
Normal, d=5, cutoff=100	7	2.66	6.95	7.48	12.93	12.39
Higher, d=5, cutoff=100	8	1.81	3.43	8.77	9.31	9.35
Normal, d=5, cutoff=60	9	2.90	7.56	8.93	15.66	14.48
Higher, d=5, cutoff=60	10	1.93	5.61	6.45	9.72	9.67
Normal, d=5, cutoff=40	11	3.13	10.82	10.21	21.27	19.91
Higher, d=5, cutoff=40	12	2.37	5.24	7.62	10.70	10.47
Normal, d=25, cutoff=100	13	3.45	8.06	4.63	8.27	8.37
Higher, d=25, cutoff=100	14	2.13	2.77	3.37	2.89	3.18
Normal, d=25, cutoff=60	15	4.45	10.56	5.94	10.69	10.79
Higher, d=25, cutoff=60	16	1.83	4.65	2.84	5.07	5.11
Normal, d=25, cutoff=40	17	5.35	13.52	7.60	13.99	14.01
Higher, d=25, cutoff=40	18	2.58	5.52	3.67	5.80	5.95
Tech 4	19	3.14	6.98	4.50	7.36	7.49

Uncertainties of Oxygen-NOx Effect from Predictive Model

By Jonathan Cohen, ICF International

Presentation at ARB Fuels Workshop
22 September, 2006

Topics

- Database is unrepresentative
- Oxygen-NOx Predictions for individual Tech 4 and Tech 5 Studies using 5 Models
  - Oxygen effects vary by model and study in size, direction, significance
- Tech 4 Dual normal and higher emitter models
  - Revised and improved
  - Fit the data statistically significantly better

PM Database is Not a Random Sample

Comparison of Test Fleet Tech 4 Normal and Higher Emitter Fractions with EMFAC 2000 Projections for 2005.						
Category	**Obs**	**Obs**	**Vehi-cles**	**Vehi-cles**	**Emissions – Test Fleet**	**Emissions - EMFAC**
	N	%	N	%	%	%
Normal (<1 g/mi)	3535	84	779	87	62	21
Higher	650	16	121	13	38	79
Total	4185	100	900	100	100	100

Statistical Models

- Latest PM database:
  - Tech 4 = 1986-1995
  - Tech 5 = 1996+, TOYOTA, AAMSUOXY
  - No outliers removed
  - Averages over repeated vehicle/fuel combinations
- Renormalize fuel parameters to mean = 0, SD = 1 for each Tech group

Statistical Models - Ctd

- Model 1. Main term OX + Other available terms. No interactions.
- Model 2. Main term OX + Other available terms. Interaction OXOX.
- Model 3. Main term OX + Other available terms. Interaction SUOX.
- Model 4. Main term OX + Other available terms. Interactions OXOX, SUOX.
- Model 5. New ARB Tech 4. All seven main terms. Interactions OXOX, SUOX, T5T5, SUSU, OLOL, ARAR, ARSU.
- Models 1-4: For each subset, OX + up to 6 more main terms arranged by fuel parameter CVs from highest to lowest. Use as many as possible where oxygen effect is estimable.

Tech 4 Studies

Study	Code	Study	Code	Study	Code
A/O-CURR	1	ARBETOH	13	EPA_ATL1	25
A/O-RVP/	2	ARBMSD96	14	EPA_ATL2	26
A/O-SULF	3	ARCO	15	EPA_PH3	27
A/O-TAME	4	ARCO5090	16	GMCONFRM	28
AO-HVT90	5	CHEVOX99	17	GMWSPA	29
AO-LOSLF	6	CHEVRON1	18	NIPER-P1	30
AO-SLFII	7	CHEVRON2	19	NIPER-P2	31
AOB17&18	8	CHEVRON3	20	UNOCAL	32
APIAROM	9	CHEVRON4	21	UNOCAL13	33
APIRVPOX	10	CHEVRON5	22	Tech 4	34
ARBATLOX	11	CHEVRON6	23	.	.
ARBATLP2	12	EPAEMFCT	24	.	.

Fig 1-1. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Studies

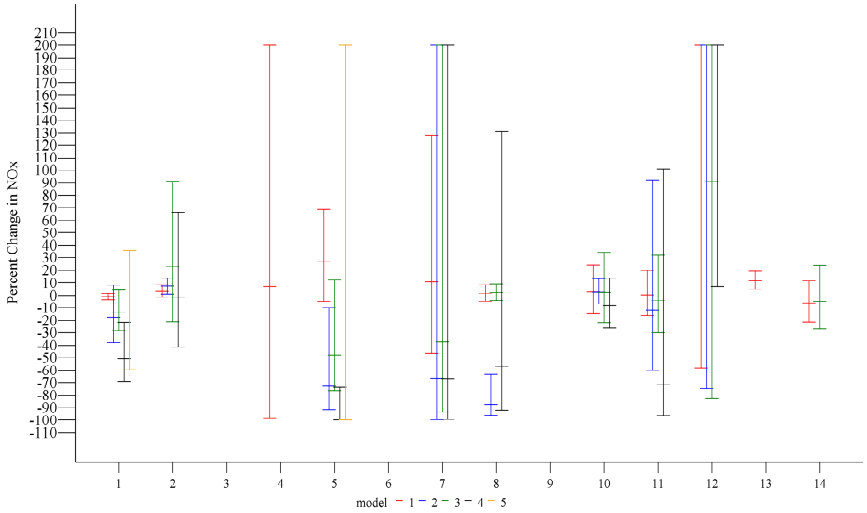


Fig 1-2. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Studies

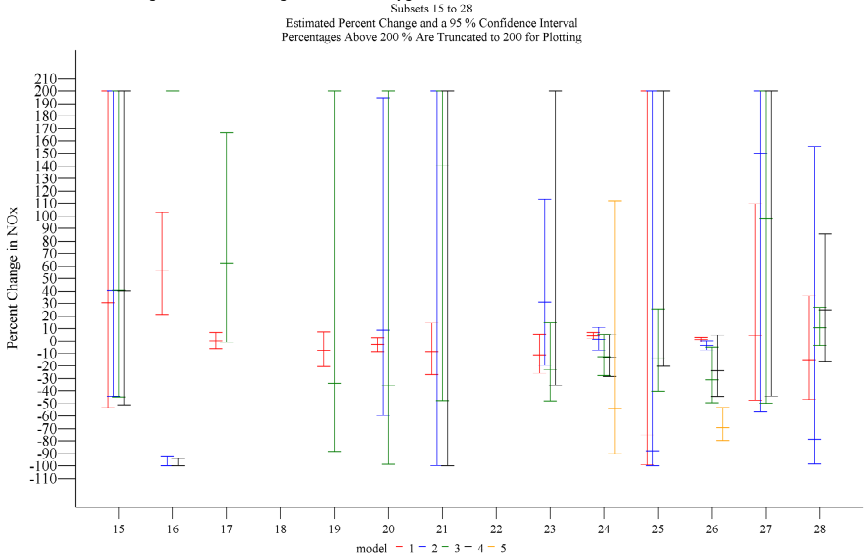
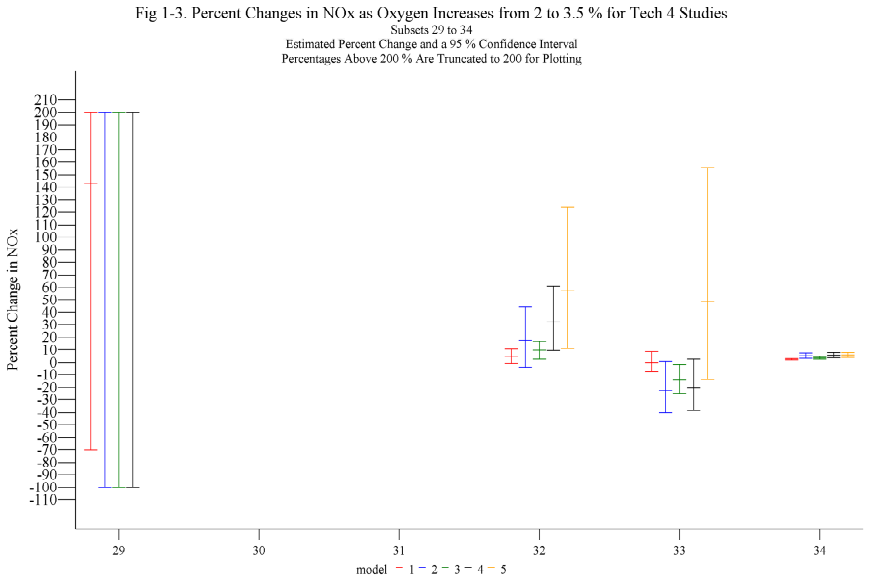


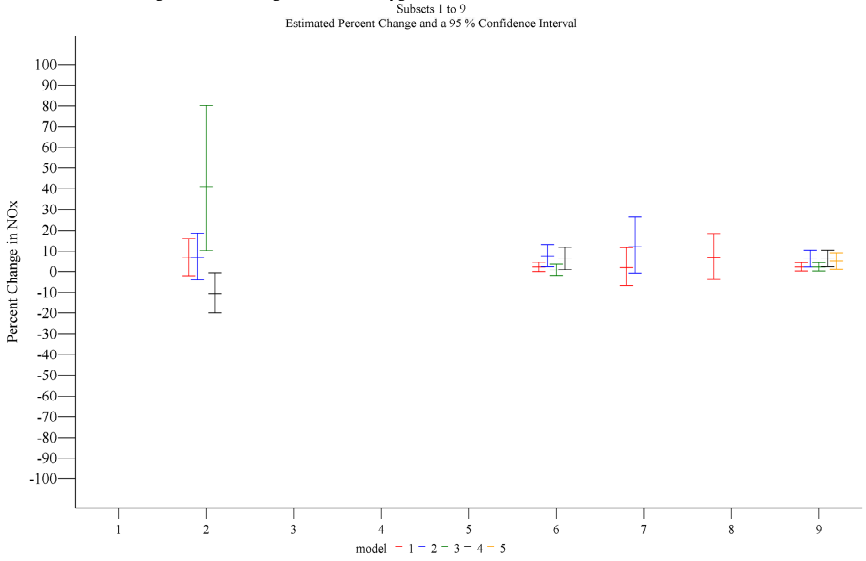
Fig 1-3. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Studies



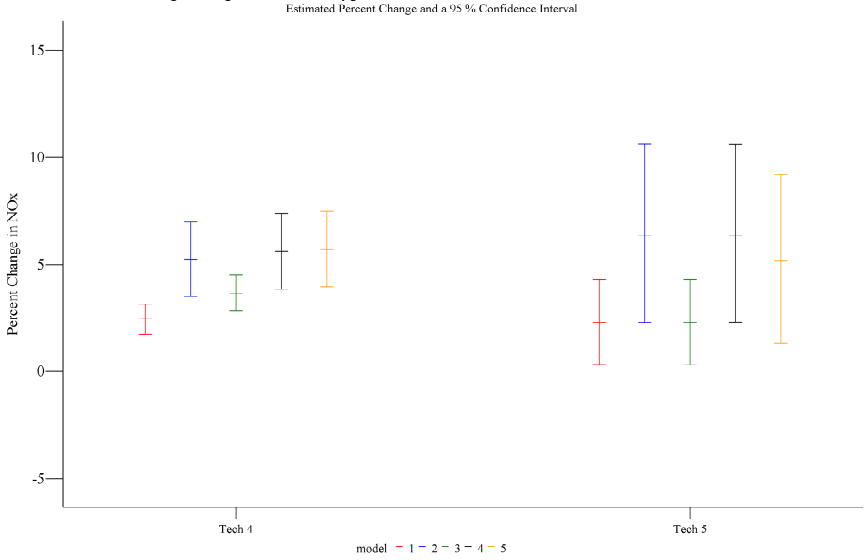
Tech 5 Studies

Study	Code
AAMALOSU	1
AAMSUOXY	2
CRCLOSUL	3
CRCLOSUO	4
CRC_E60	5
CRC_E67	6
EXXONMOBIL	7
TOYOTA	8
Tech 5	9

Fig 2. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 5 Studies



Percentage Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 and Tech 5 Models



Summary 1

- Database is not a random sample
- Higher-emitting vehicles under-represented
- Oxygen effects are inconsistent across studies, varying in direction and statistical significance
- Oxygen effects vary across models
- Predictive Model ignores uncertainties in database, model formulation, and model coefficients in determining compliance: Uses a point estimate from one model

Tech 4 Dual Models: Higher and Normal Emitters

- For each Tech 4 vehicle, find emissions on closest fuel to Auto/Oil Fuel A:
  "Distance" = $\{RVP(F) - RVP(A)\}^2 / Var(RVP) + \{SU(F) - SU(A)\}^2 / Var(SU) + \ldots$
- Fuel A = most frequent base fuel in Tech 4
- Previous approach was to average emissions, potentially biasing "higher" emitters towards higher emitting fuels
- d = 0: Only use 86 vehicles tested on A.
- d = 5: Distance <= 5. 248 vehicles.
- d = 25: Distance <= 25. All 900 vehicles.

Tech 4 Dual Models: Cutoffs

- Vehicle NOx emissions (closest fuel):
  - <= Cutoff "Normal"
  - > Cutoff "Higher"
- Cutoff = 100 %, 60 % or 40 % of 1 g/mile NOx std
- 100 %: Higher = EMFAC Moderate, High, Very High, Super
- 60 %, 40 %: Gave two best-fitting models in previous analyses.

Tech 4 Dual Models: Codes

Study	Code	Study	Code
Normal, d=0, cutoff=100	1	Normal, d=5, cutoff=40	11
Higher, d=0, cutoff=100	2	Higher, d=5, cutoff=40	12
Normal, d=0, cutoff=60	3	Normal, d=25, cutoff=100	13
Higher, d=0, cutoff=60	4	Higher, d=25, cutoff=100	14
Normal, d=0, cutoff=40	5	Normal, d=25, cutoff=60	15
Higher, d=0, cutoff=40	6	Higher, d=25, cutoff=60	16
Normal, d=5, cutoff=100	7	Normal, d=25, cutoff=40	17
Higher, d=5, cutoff=100	8	Higher, d=25, cutoff=40	18
Normal, d=5, cutoff=60	9	Tech 4	19
Higher, d=5, cutoff=60	10	.	.

Fig 3-1. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Normal and Higher Emitters

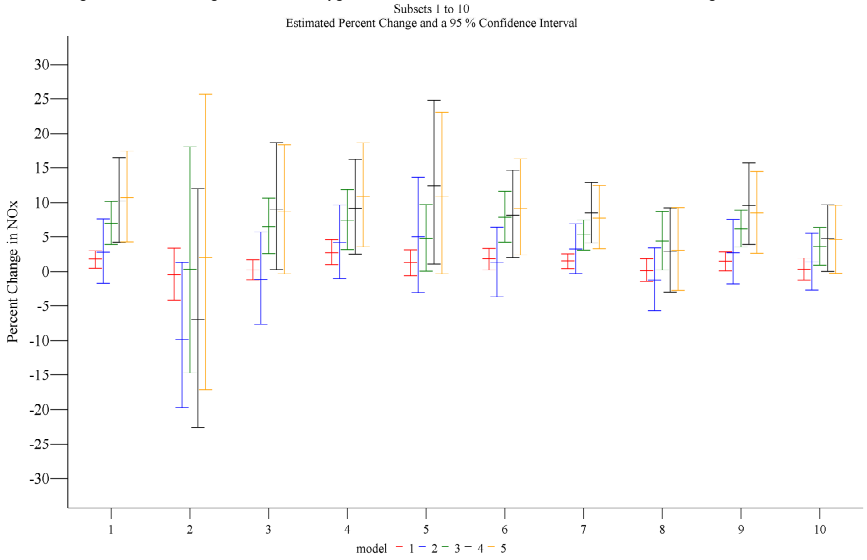


Fig 3-2. Percent Changes in NOx as Oxygen Increases from 2 to 3.5 % for Tech 4 Normal and Higher Emitters

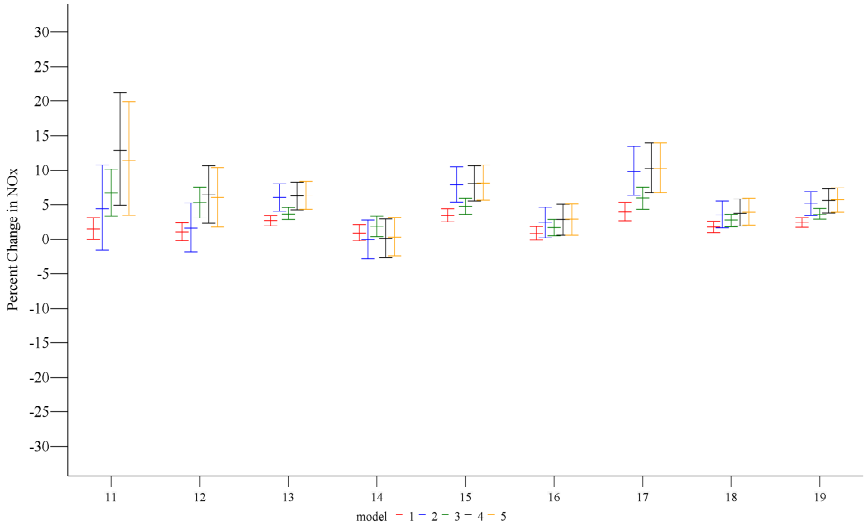
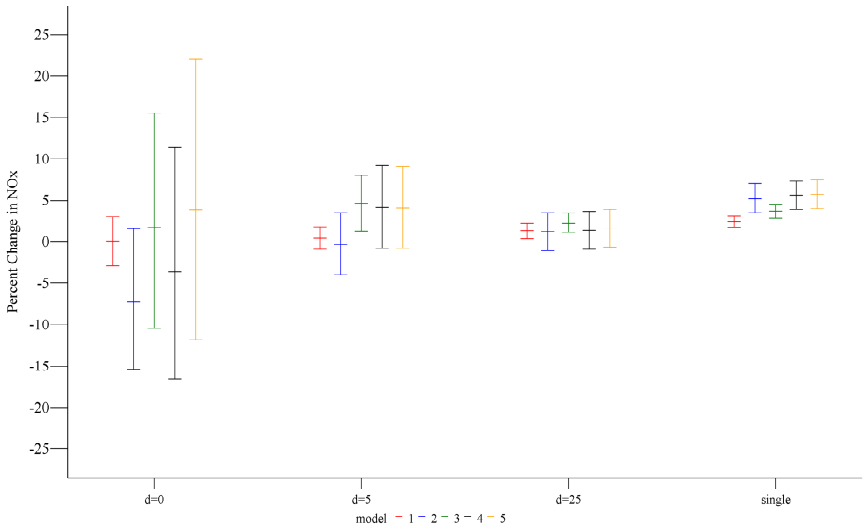


Fig 4. Weighted Averages for Dual and Single Models for 2005 based on EMFAC 2000
Dual Model Cutoff = 1 g/mile
Estimated Percent Change and a 95 % Confidence Interval



Summary 2

- Dual models fit the data statistically significantly better
- Best-fitting of three cutpoints was 60 %
- Higher emitters respond less to oxygen than normal emitters
- Ideal model would have multiple or infinitely many cutpoints – dual model is an approximation
- Possible “engineering” explanation: catalyst aging; fresher catalysts are less stable

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D-3) DEVELOPMENT OF EVAPORATIVE EMISSIONS MODELS

Background

It has been well established that the presence of ethanol increases the vapor pressure of gasoline. This RVP increase increases evaporative emissions, including permeation. To investigate the impact of ethanol on permeation emissions, the ARB co-funded a research study with the CRC to assess the magnitude of the permeation emissions associated with the use of ethanol in gasoline (CRC E-65 Study).

Based on the study results, staff calculated the increase in evaporative emissions from on-road motor vehicles (GVW<10,000 lbs.) due to the presence of ethanol in gasoline to be about 12.1 tpd of hydrocarbons in 2015. In late 2006, ARB released the latest update to California's on-road motor vehicle emissions model, EMFAC2007. This model was updated to include permeation emissions.

Staff used EMFAC2007 to estimate evaporative emissions by process (diurnal/resting loss, hot soak, and running loss), including permeation emissions. Permeation emissions are highly affected by ambient temperature, so it is important to use a temperature profile that recognizes this relationship. For this analysis, EMFAC2007 used the temperature profiles that occur when the California 8-hour ozone standard was exceeded. In general, the California 8-hour ozone temperature profiles are about two to three degrees Fahrenheit higher than the default temperature profile included in EMFAC2007.

Table 1 presents the evaporative emissions at various RVPs for two fuels, ethanol and MTBE blended gasolines, based on California 8-hour ozone temperature. Staff assumed evaporative emissions from non-oxygenated gasoline are the same as MTBE fuel. In addition, staff also assumes that permeation increase is constant with RVP, as shown in the last column of the table

Regression Equations

Staff developed regression equation for each of the evaporative process as a function of RVP. This regression equation was developed using MS Excel. Staff tried two functional forms (exponential and linear) that relate evaporative emission (tpd) as dependent variable to RVP (psi) as independent variable, and found that linear function seemed to give the best fit to the data.

Figures 1-3 show individual regression lines and equations. As can be seen in these figures, each evaporative process is represented by two parallel lines for the three fuels. The separation between the two lines indicates the increase in permeation emissions associated with ethanol in gasoline. For example, ethanol permeation increase in diurnal and resting loss is about 9 tpd relative to MTBE/non-oxy fuel, as shown in Figure 1.

Table 1: Evaporative Emissions by RVP

2015 Statewide (GVW < 10,000 lbs.)

RVP (psi)	Evaporative Emissions (tpd)								
	DI / Rest Loss		Hot Soak		Running Loss		T o t a l		EtOH Perm Incr*
	EtOH	MTBE	EtOH	MTBE	EtOH	MTBE	EtOH	MTBE	
6.6	68.2	59.2	39.2	38.1	106.8	104.9	214.3	202.1	12.1
6.8	69.0	59.9	40.0	38.9	108.8	106.8	217.8	205.7	12.1
7.0	69.7	60.6	40.9	39.8	110.7	108.8	221.4	209.2	12.1
7.2	70.5	61.4	41.8	40.7	112.7	110.7	225.0	212.9	12.1

Source: EMFAC 2007 (Vehicles MY 1965-2015), CA-8 Hour Ozone Day Temperature
*****Ethanol permeation increase is computed as the difference between total evaporative emissions of ethanol and MTBE fuel. The results may differ slightly from what are shown in the last column of the table due to rounding.

Fig 1. Diurnal / Resting Loss Regression Line

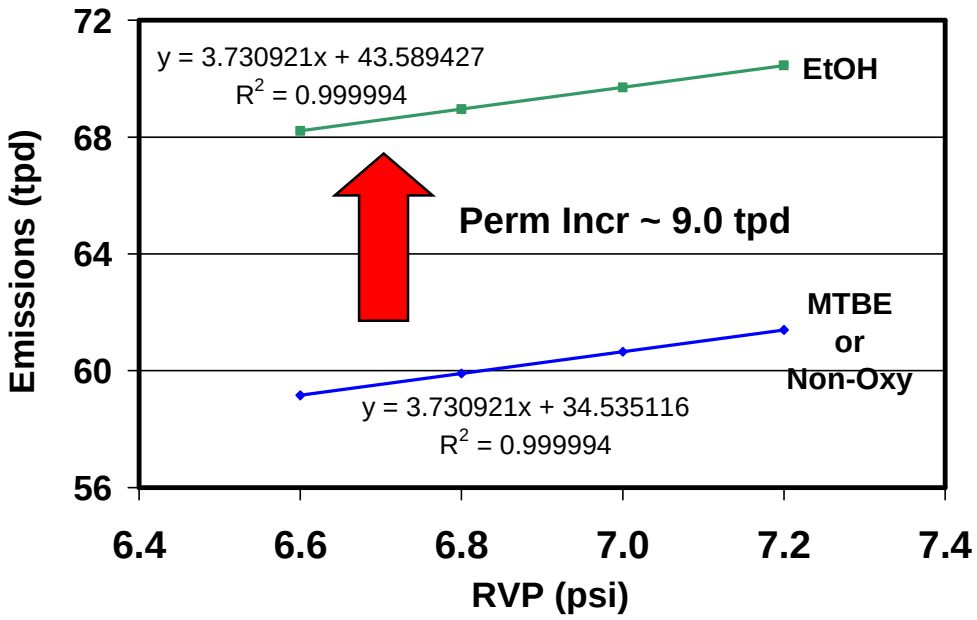


Fig 2. Hot Soak Regression Line

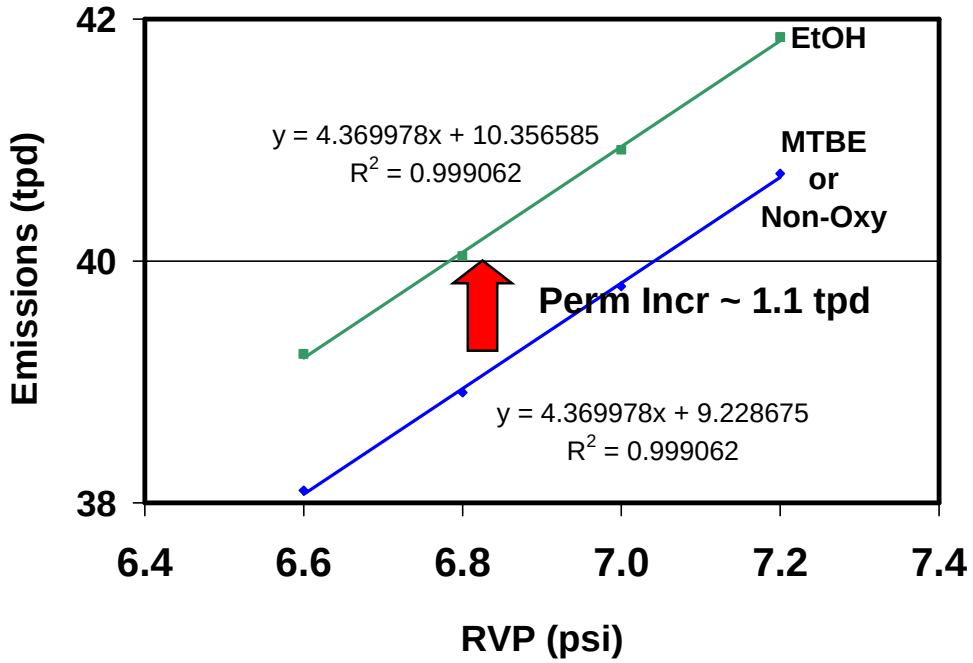
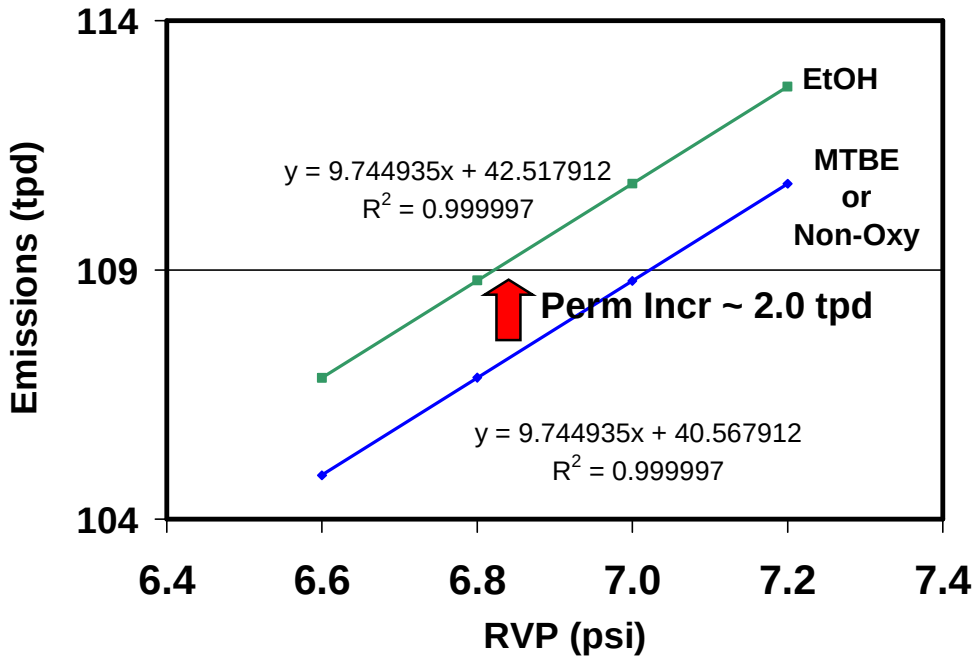


Fig 3. Running Loss Regression Line



Using these equations, the predicted percent change in evaporative emissions can be estimated as follows:

$$\%CE_j = (E_{Cand} / E_{Ref})_j * 100\%$$

Where,

$\%\ CE_j$ = the predicted percent change in evaporative process j (diurnal/rest, hot soak, or running loss);
E_{Cand} = candidate fuel evaporative emissions (tpd); and
E_{Ref} = reference fuel evaporative emissions (tpd), with RVP sets to 7.0 psi for ethanol candidate fuel and RVP equals to 6.9 psi for non-oxygenated fuel.

For instance, the predicted percent change in diurnal/resting process associated with a 6.8 psi RVP ethanol gasoline is computed as follows:

$$\%CE_{diurnal/rest} = (3.730921*6.8 + 43.589427) / (3.730921*7.0 + 43.589427)*100\%$$

Similarly, the predicted percent change in hot soak and running loss can be computed using the corresponding equation.

Emissions Weight and Reactivity Adjustment

Once the predicted percent change associated with each evaporative process is established, staff used emissions weight and reactivity adjustment factors to estimate the ozone-forming potential of the evaporative emissions. These factors are shown in Tables 2 (a) and 2 (b), respectively.

Table 2 (a): Emissions Weight

2015 Statewide, (GVW<10,000 lbs.)

Evaporative Process	Weight Factors
Diurnal	0.291
Hot Soak	0.189
Running Loss	0.519
T o t a l*	1.000

Source: EMFAC2007
*Total may not add up to1.000 due to rounding errors

Table 2 (b): Reactivity Adjustment Factors

Evaporative Process	Average Specific Reactivity (tons O_3/ton TOG)
Diurnal	2.74
Hot Soak	3.12
Running Loss	2.73

As can be seen in the above tables, running loss contributes about 52 percent of evaporative emission in 2015, but hot soak process has the highest ozone forming potential. These factors are used to estimate the overall ozone forming potential (OFP) is the sum of individual OFP evaporative processes, as described in the following equation:

$$\%OFP_{evap} = \Sigma_j (\%CE_j * EW_j * MIR_j)$$

Where,

EW_j = emissions weight of evaporative process j (diurnal/rest, hot soak, or running loss); and

MIR_j = reactivity adjustment factor of evaporative process j.

A more detailed discussion of the subject is given in “California Procedures for Evaluating Alternative Specifications for Phase 3 Reformulated Gasoline Using the California Predictive Model” (Appendix A).

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D-4) COMMENTS FROM EXPERT REVIEWERS