Final Report

Humidity and Temperature Effects on On-road and Off-road Emissions and Ozone Formation (HARC Project H8B)

Prepared for

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ENVIRON also acknowledges the technical work performed by Southwest Research Institute, whose literature review and engineering calculations and judgments detailed in Appendices A and B provided the basis for the emission adjustments used in this work.

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1. INTRODUCTION

The effect of ambient humidity and temperature on the performance and emissions from internal combustion engines, including spark-ignition (SI) engines (gasoline, LPG and natural gas engines) and compression ignition (CI) or diesel engines, has been known for many years. The historical data indicate that higher humidity results in lower NOx emissions. Likewise, higher temperatures have historically been associated with higher emissions except during the cold start for light-duty vehicles when emission control devices and other engine controls may not function properly. Once the engine has warmed up though, higher temperatures result in higher NOx emissions.

The effect of humidity and temperature has been included in nearly all emission measurement methods calculations whether tested in the laboratory or in the field. The codified humidity and temperature corrections for NOx emissions from gasoline and diesel fueled engines are described in the U.S. Code of Federal Regulations (CFR) 86-345-79 and reprised in the International Standard ISO 8178-1 used to correct the available field measurements of commercial marine engines.

Emission inventories, however, have not accounted for humidity and temperature adjustments except for light-duty on-road vehicle emissions estimates in MOBILE6, and that adjustment primarily includes the effect of ambient conditions on air conditioning loads on the engine. The effect of temperature and humidity has not been included in the emission models, MOBILE6 for heavy-duty vehicles and NONROAD for off-road equipment, or for locomotive or commercial marine engine emissions even though the emission data used in the development of emission factors have been adjusted for temperature and humidity using the official adjustment equations in the CFR.

The technical approach of this work was to define the effect of ambient conditions on NOx emissions for on-road vehicles and off-road engines or equipment. This effect was then used to adjust the emission estimates for the Houston-Galveston nonattainment area (HGA) on the portion of the emission inventory consistent with the engine technology by the hourly and spatial ambient temperature and humidity conditions.

While the emissions adjustments described in this work may be considered significant, with a daily 5 to 10% change in NOx emissions for heavy-duty on-road vehicles and off-road equipment, the overall change in emissions was not large in absolute terms compared with all sources in the region. Likewise, the change in the predicted ozone is small both in the year 2000 base case and the 2007 future year projections.

Section 2 describes the review, development, and use of the ambient humidity and temperature emission adjustments used in this work. This section refers to the literature review and engineering analysis performed by Southwest Research Institute provided as complete reports in Appendices A and B. Section 3 describes the effect the adjustments have on predicted ambient ozone levels in 2007 and ozone model performance in 2000.

2. DEVELOPMENT OF HUMIDITY AND TEMPERATURE CORRECTION FACTORS

Emission regulations continue to place additional restrictions on urban areas trying to achieve ambient air quality standards. Although ambient air quality standards are national, achieving the standards is a regional problem delegated to the states. However, the certification procedures for on-road and off-road spark-ignited engines are standardized without regard for regional variation in ambient conditions like temperature and humidity. As early as 1970 (Brown et al., 1970), it was recognized that the concentration of oxides of nitrogen (NO_x) in engine exhaust is significantly affected by the thermodynamic conditions of the intake air. Specifically, the intake air temperature and humidity have the dominant effects (Brown et al., 1970, Manos et al. 1972, Krause et al. 1971). Because of these sensitivities, it is reasonable to assume regional variations in temperature and humidity can significantly impact engine-out emission levels. Mobile source emissions models such as the EPA's MOBILE and NONROAD (Glover et al. 1999, EPA, 2002, ARB, 2000) have been developed to account for pollutants attributed to both on-road and off-road mobile sources. These models often use local information including fuels, regional temperature and humidity for some, but not all, categories of engines types to adjust the emissions inventory.

Historically, the impact of ambient temperature and humidity on emissions was of interest because it was difficult to make comparisons of the NO_x emissions from engines tested at different locations and/or with variations in the ambient conditions. In an effort to allow day-to-day and location-to-location comparisons, various correction factors have been developed. The goal for all of these correction factors has been to standardize the NO_x emissions to reference conditions, but these correction factors can also be used to adjust emissions inventory models to more accurately predict ambient air quality. To improve the air quality modeling, it is appropriate to account for regional differences by including the effect of ambient conditions on emissions rates, particularly NO_x emissions, a major contributor to ambient air ozone levels.

This section provides an overview of the literature search results of studies for humidity and temperature effects on NOx emissions for CI and SI engines. Recommendations are provided for a set of NOx correction factor equations for CI and SI engines by application, technology, and fuel types.

The NOx correction factor to account for humidity and temperature is defined as the KNOx variable in equation (1). The NOx emission at the reference condition multiplied by the correction factor yields the best estimate of the in-use emissions. The reference conditions are not consistent across all the correction factor equations.

$$\text{NOx-actual} = \text{KNOx} * \text{NOx-reference} \qquad (1)$$

The correction factor equations vary by engine type and technology, and the best estimates are described for each type. Southwest Research Institute (SwRI, 2004) reviewed the literature and used engine thermodynamic models to recommend different correction factor equations by engine type (compression-ignition in Appendix A, and spark-ignition in Appendix B) and by technology within the two engine types.

Compression-Ignition (Diesel) Engines

The review work performed by SwRI (2004) provided further evidence that the humidity levels do affect the emission levels in late model diesel engines. In general, the results indicated that emission levels could be corrected by applying a NOx correction factor, KNOx, to a reference NOx emissions value as shown in Equation 2. This NOx correction algorithm is comparable but more straightforward than those correction equations found in the Code of Federal Regulations (CFR) used to correct laboratory emissions estimates. The NOx correction factor is a function of humidity and temperature; the constant coefficients in Equation 2 vary by application and technology types for the engine.

$$\text{KNOx} = 1.0 + [0.004460 \times (\text{TEMP} - 25)] - [0.018708 \times (\text{HUMID} - 10.71)] \qquad (2)$$

where TEMP is temperature in ^{o}C and HUMID is humidity in grams of water per kilogram of dry air

As part of this work, a set of equations to estimate emission adjustments, KNOx, were used to correct emission rates for each engine type.

<u>On-Road Diesel Vehicles</u>

Pre-1994: Naturally Aspirated Diesel Engines

English Units:

$$\text{KNOx} = 1 + 0.00076\ (T - 85) - 0.00216\ (H - 75) \qquad (3)$$

(Units of T in ^{o}F, and H in grains per pound of dry air)

SI Units:

$$\text{KNOx} = 1 + 0.001368\ (T - 29.444) - 0.01512\ (H - 10.71) \qquad (3a)$$

(Adjusted to consistent units of ^{o}C and grams per kg of dry air)

The correction algorithm is essentially similar to the EPA correction factor without the Fuel/Air ratio dependence. This eliminates the requirement for determining the Fuel/Air ratio of the fleet.

Post 1994: Turbocharged Diesel Engines

$$\text{KNOx} = 1 + 0.00446\ (T - 25) - 0.018708\ (H - 10.71) \qquad (4)$$

where *T = ambient temperature, ^{o}C*
H = ambient humidity, g H2O/kg of dry air

The effect of these adjustments can also be seen in Figure 2-1 for natural aspirated engines following equation 3, and in Figure 2-2 for turbocharged engines following equation 4.

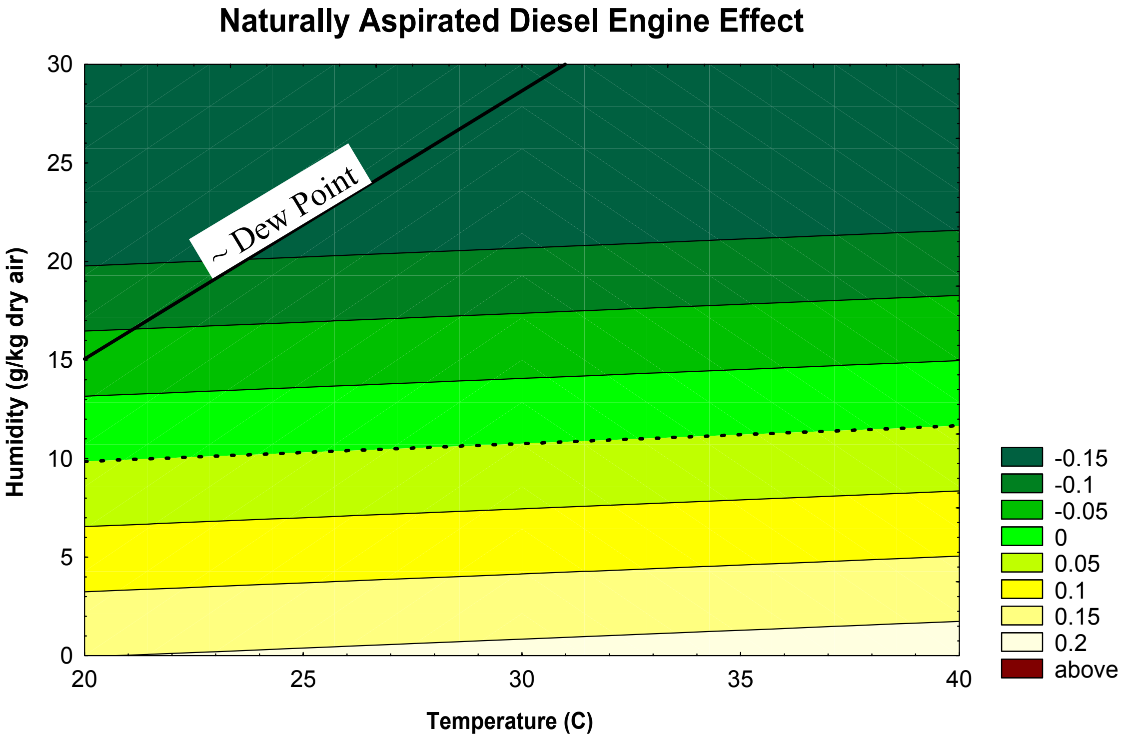


Figure 2-1. NOx adjustment (fractional change, 1 - KNOx) from equation 3. (Dotted line is no adjustment or KNOx =1).

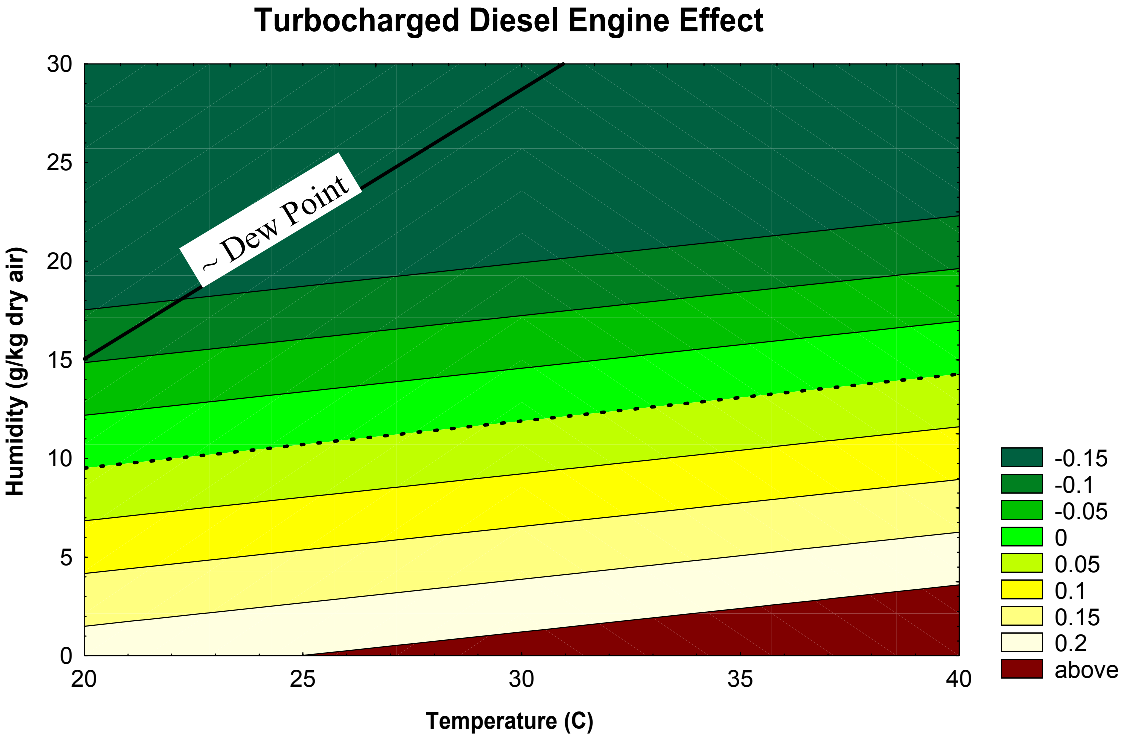


Figure 2-2. NOx adjustment (fractional change, 1 - KNOx) from equation 4. (Dotted line is no adjustment or KNOx =1).

Off-Road Diesel Engines

Naturally Aspirated Diesel Engines for Construction/Farm Equipment

Similar to Pre 1994 on-road vehicles, Equation 3 or 3a was recommended.

Turbocharged and Charge-Cooled Diesel Engines for Construction/Farm Equipment

Similar to Post 1994 on-road vehicles, Equation 4 was recommended.

Railroad and Marine Diesel Engines

$$KNOx = 1 / (K_H K_T) \qquad (5)$$

$$\text{where } K_H = 1989.6/(85.444 + 2219.426 \exp(-0.0143 H))$$
$$K_T = 1 / (1 - 0.017 (30 - T))$$

The effect of these adjustments can also be seen in Figure 2-3 for larger locomotive and commercial marine engines.

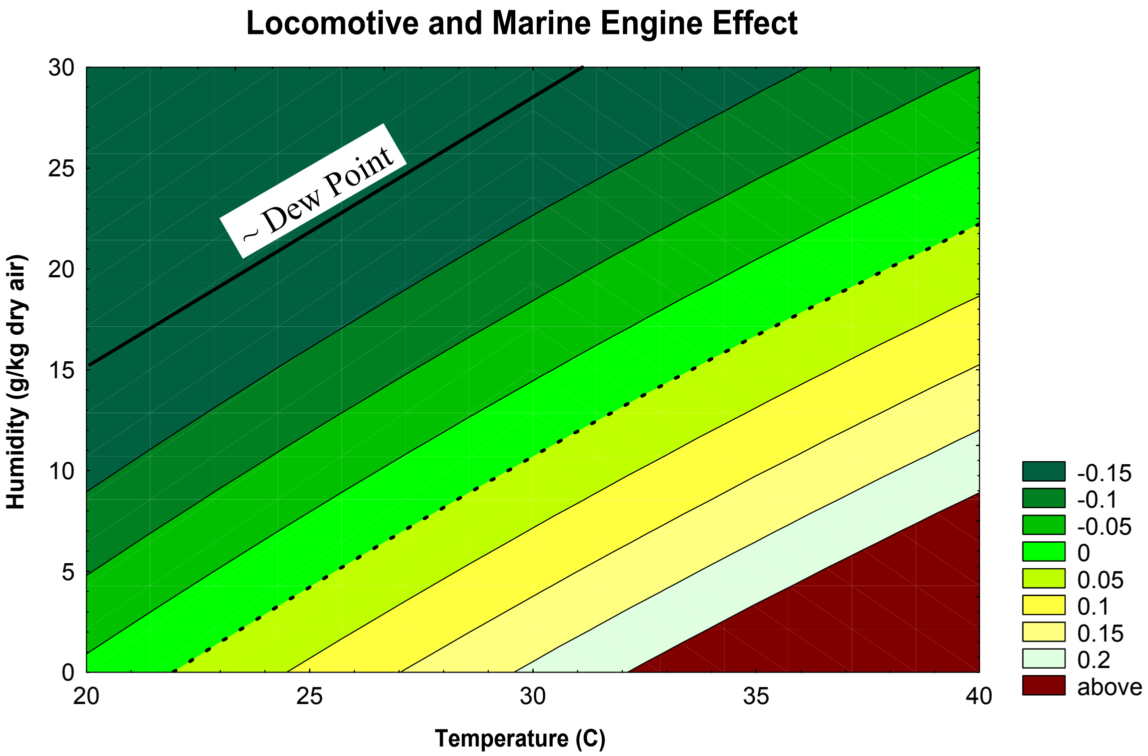


Figure 2-3. NOx adjustment (fractional change, 1 - KNOx) from equation 5. (Dotted line is no adjustment or KNOx =1).

Spark-Ignition (Gasoline, LPG and NG) Engines

All of the current humidity correction factors for NO_X for SI engines were based on historical data taken in 1971 and 1972. Some of the engines today are more technically advanced, incorporating port or throttle-body fuel injection, air-fuel ratio feedback, exhaust aftertreatment, and knock detection. While many off-road vehicles do not have all of these features, this technology is becoming more prevalent with the implementation of Federal rulemakings beginning with model year 2004. SwRI's (2004) analysis conducted indicated that the historical correction factors do not adequately account for operating cycles with higher load factors, or advanced technologies such as A/F control and knock detection. No engine test data were found documenting humidity effects for these additional variables.

SwRI's (2004) engine model results showed these effects to be significant and the results were used to modify the historical correction procedures. While SwRI recommended some NOx correction factor algorithms for SI engines as follows, SwRI recommended engine testing to quantify the effects for different engine/vehicle classes, if a more rigorous approach is desired.

The recommended equation to adjust standardized emissions for a **carbureted heavy-duty on-road or off-road (above 19kW) engine** under non-standard inlet air conditions takes the following form, with the adjustment shown in Figure 2-4:

$$KNOx = 1 + 0.0022\ (T - 25) - 0.0280\ (H - 10.71) \qquad (6)$$

where:
T = Temperature of the inlet air [^oC]
H =Absolute humidity of the inlet air [g of H_2O/kg of dry air]

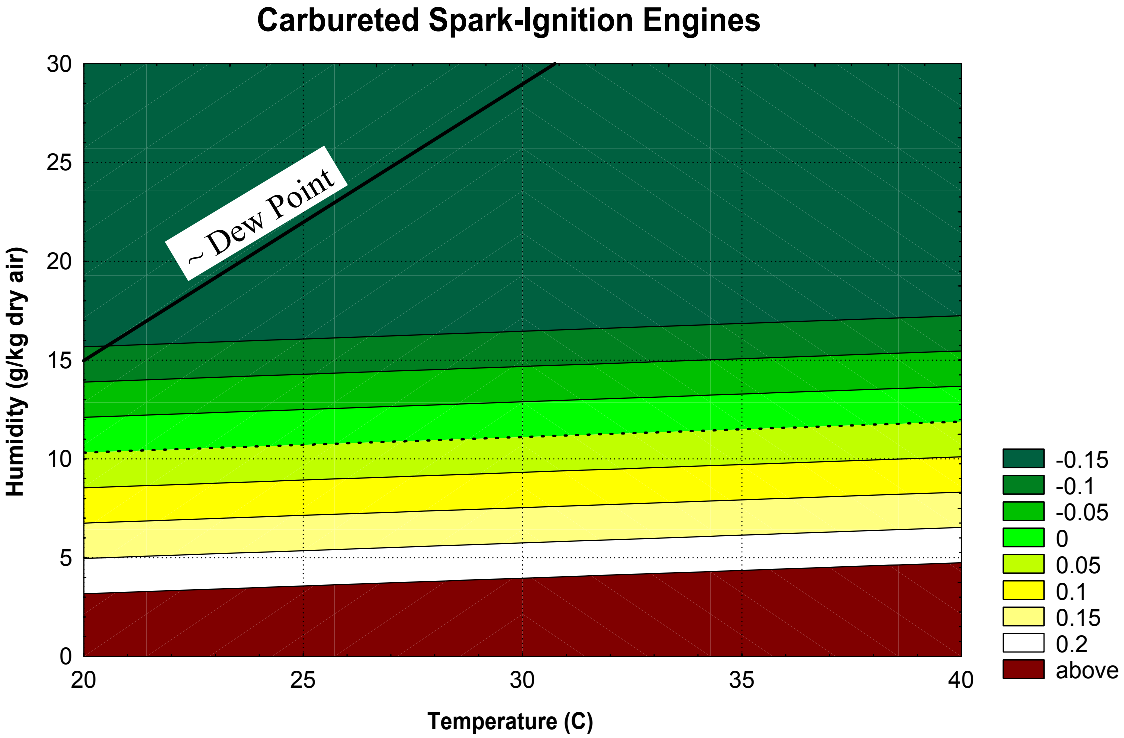


Figure 2-4. NOx adjustment (fractional change, 1 - KNOx) from equation 6. (Dotted line is no adjustment or KNOx =1).

For **heavy-duty on-road or off-road (above 19kW) spark-ignition engines** that use a 3-way catalyst (A/F control, typically with port fuel injectors), the recommended NO_x correction equation is as follows with the adjustment shown in Figure 2-5:

$$\text{KNOx} = 1 - 0.0232\ (H - 10.71) \qquad (7)$$

with no correction for ambient temperature.

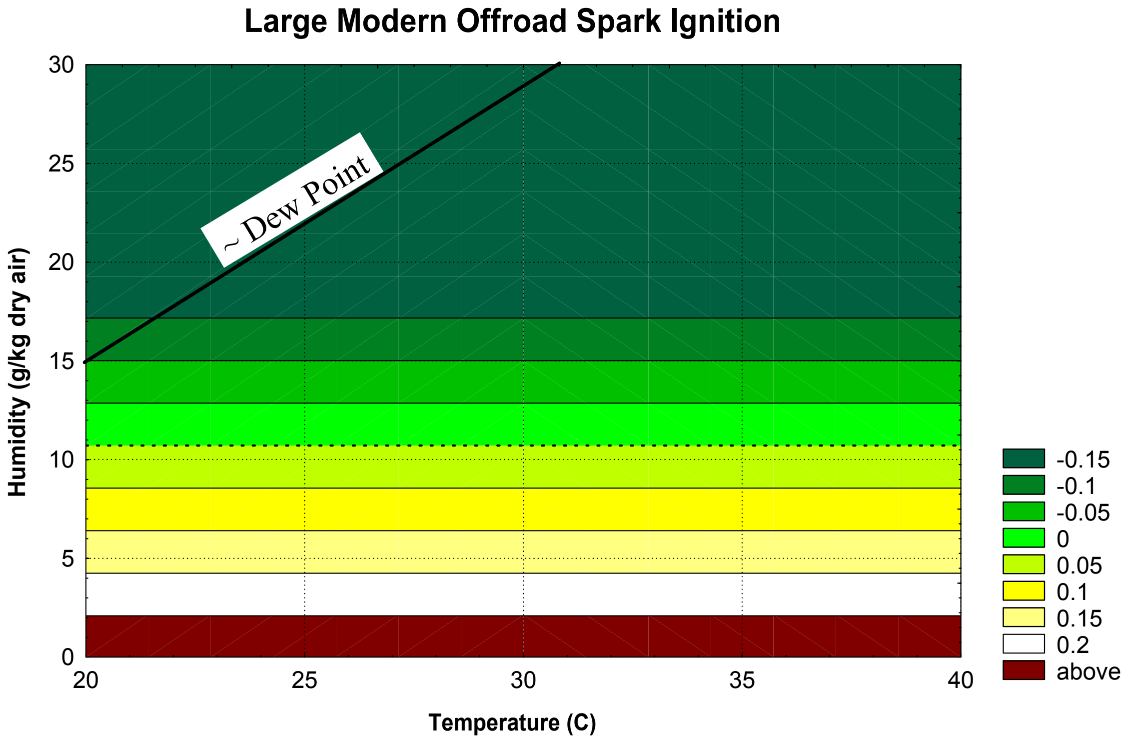


Figure 2-5. NOx adjustment (fractional change, 1 - KNOx) from equation 7. (Dotted line is no adjustment or KNOx =1).

For **light-duty, spark-ignition engines**, the recommended practice is the procedure used in MOBILE6, which can be approximated by Equation 8, except for load adjustments due to increased use of air conditioning compressors during hot and humid weather.

$$\begin{aligned} \text{KNOx} &= 1.2 \text{ if } H_a \# 20 \\ &= (-0.004\ H_a + 1.28) \text{ if } 20 \ \$ \ H_a \# 120 \qquad (8) \\ &= 0.8 \text{ if } H_a \ \$ \ 120 \end{aligned}$$

where:
H_a = Absolute humidity of the inlet air [grains/lb]

For **small off-road, spark-ignition engines (< 19kW)**, the recommended practice is

$$\text{KNOx} = 1 - (0.546 / \text{AFR})\ (H - 10.71) \qquad (9)$$

where:
AFR = Air-fuel ratio of the engine
H = Absolute humidity of the inlet air [g/kg dry air]

Application of Correction Factors

In order to determine the proper emissions adjustment, the fraction of emissions for each engine technology type was estimated for each on-road heavy-duty vehicle category and off-road source category code (SCC, used to identify off-road equipment types). The engine types used in equipment varied by engine size and model year grouping, both of which could affect the technology used in such engines. For on-road heavy-duty diesel the model year of 1994 was used to divide the technology types for application of different adjustment factors:

On-road Heavy-Duty Diesel Adjustment
<1994 Model Years; 100% Equation 3
1994 and later Model Years; 100% Equation 4

For off-road diesel engines other than locomotive and marine engines, the primary deciding factor was whether the engine was turbocharged or not. According to EPA (1998), the fraction of turbocharged engines has been and will be associated with the size of the engine. For the power category of 50 to 100 horsepower, EPA estimated none were turbocharged, but the latest information from EPA (2003) indicates that approximately 10% of these engines in the 1998 – 2002 model year certification data were turbocharged. These assumptions were used when applying the NOx correction factors as follows:

Off-road (Latest NONROAD model)
<50 hp; 100% Equation-3
50-100 hp; 10% Equation-4 & 90% Equation 3
100-175 hp; 58% Equation-4 & 42% Equation 3
>175 hp; 100% Equation-4

The SI engine definitions are straightforward in that the emission standard forces the technology definition of equation (7) for large (>19kW) off-road engines in model years 2004 and later, and model years 2005 and later for on-road SI heavy-duty vehicles. Earlier heavy-duty on and off-road engine emissions were given the equation (6) adjustment. Smaller off-road 4-stroke SI engine emissions were given the equation (9) adjustment, with no adjustment to 2-stroke SI engine emissions.

The emission inventory was then divided into groups associated with each adjustment equation described above. As demonstrated in the results section, the adjustment magnitude does not vary much between each equation, so the uncertainty in defining the fraction of the emission inventory associated with each technology type adds much less uncertainty to the overall estimates than it appears.

For on-road vehicles, the model year is the defining characteristic. While the actual emissions inventory was developed using a detailed link level analysis (small sections of the road network) with specific emissions for each link, it was not possible to use this inventory analysis to delineate by model year. So a single MOBILE6 run with a distribution of speeds and roadway facility reflecting average conditions was developed that estimated emissions well within 10 percent of the link level estimates. This run was then used to determine the fraction of the emission inventory by model year to apply the correction of each equation.

For off-road equipment both power level and model year are the defining characteristics. The NONROAD2002 model was used to estimate the emission inventory fractions by SCC (individual equipment types grouped to general off-road categories) according to the description above.

EMISSION INVENTORY RESULTS

ENVIRON and the Texas Commission on Environmental Quality (TCEQ) jointly modified the 8-county Houston-Galveston nonattainment area (HGA) emission inventory to reflect the best estimate of humidity and temperature corrections to the in-use emissions inventory. A new emissions processing software tool (CNTRLHR, a modified version of CNTRLEM) was developed by ENVIRON for this work to apply emission control factors by hour, county, and emission source. TCEQ then used this software to modify their emission inventory to reflect the conditions experienced during their ozone-modeling episode.

Average hourly county-level conditions for the modeling episode were used to estimate the adjustment to the emissions. The hourly ambient conditions were derived from data recorded at monitors operated by the National Weather Service, TCEQ air quality stations, and the Conrad Blucher Institute coastal stations for each county within the HGA. The county and hourly ambient conditions estimates used in the NOx adjustment were identical to those used in MOBILE6 when developing the link level on-road emissions inventory.

An example of the adjustment for hourly conditions for one modeling day is provided for diesel engines in Figures 2-6 through 2-8. The NOx emissions are reduced for late night and early morning when the temperature is low, and are relatively unchanged for mid-day. The data reflect the most important county for emissions (Harris), a wet county (Galveston), and a dry county (Montgomery). Emissions can be seen to vary spatially, where the coastal counties experience higher humidity (absolute humidity in mixing ratio units of grams water per kilogram of dry air) and therefore lower NOx emission rates.

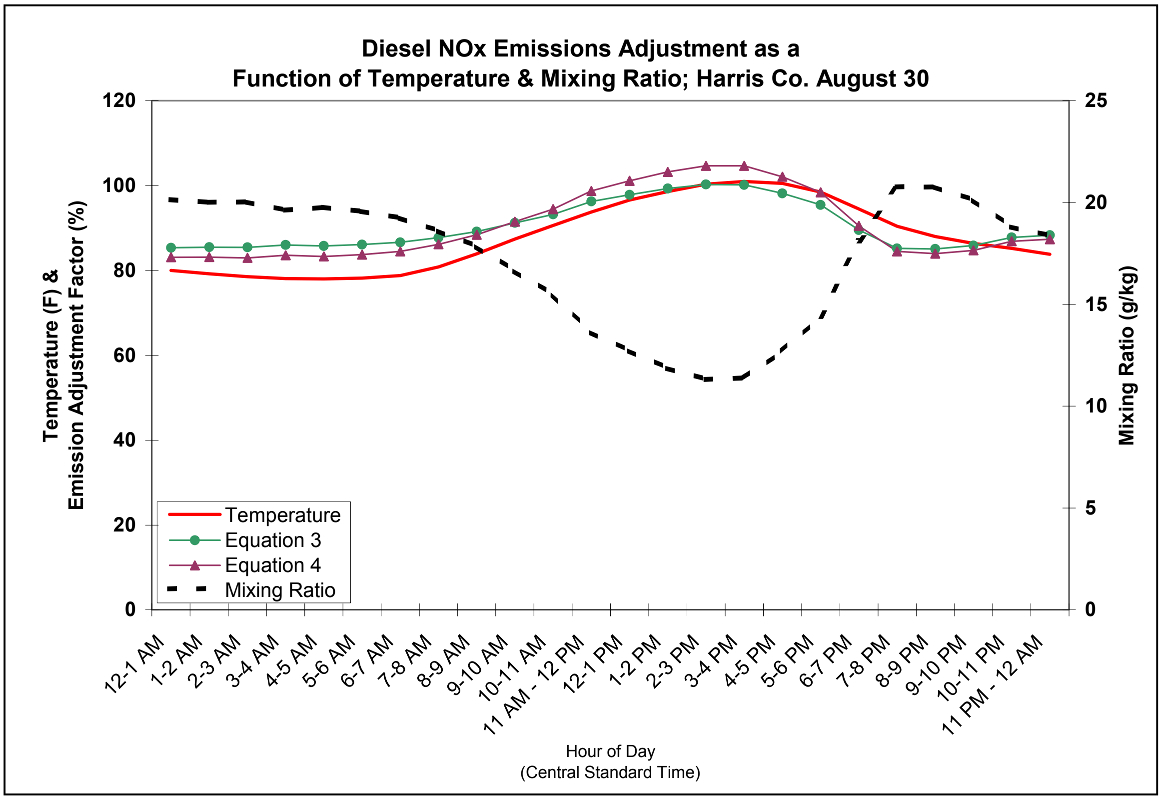


Figure 2-6. Diesel engine emissions adjustments for Harris County on August 30.

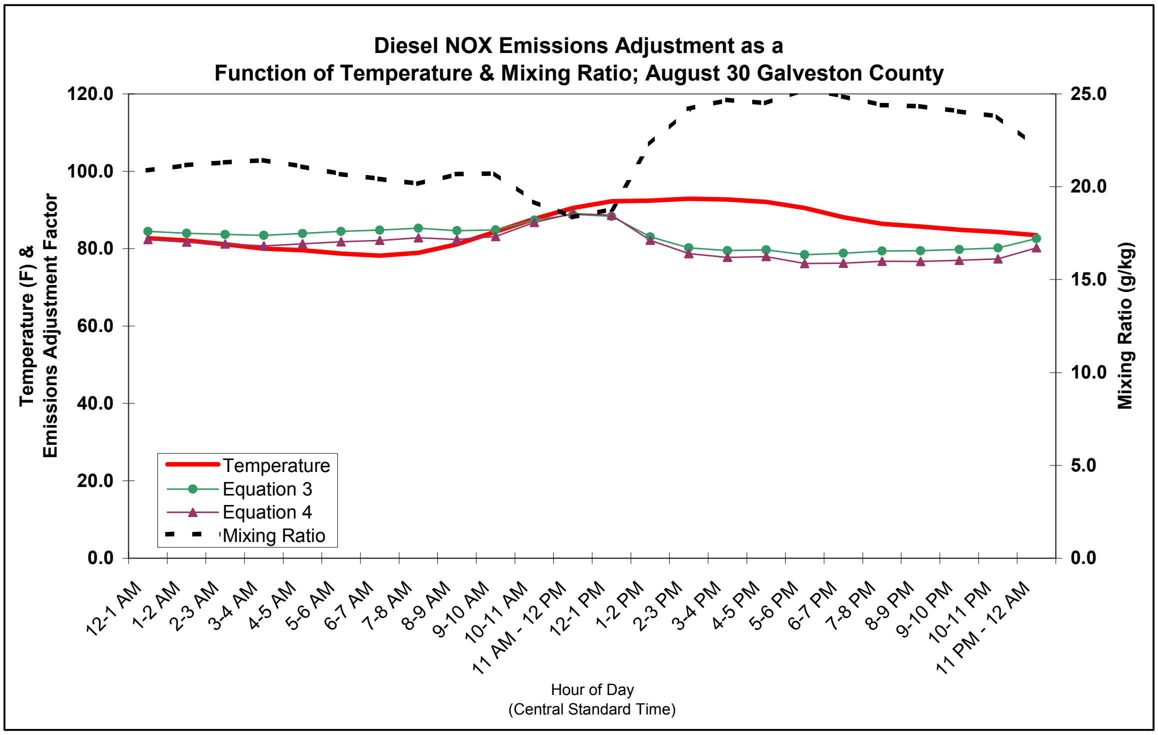


Figure 2-7. Diesel engine emissions adjustments for Galveston County on August 30.

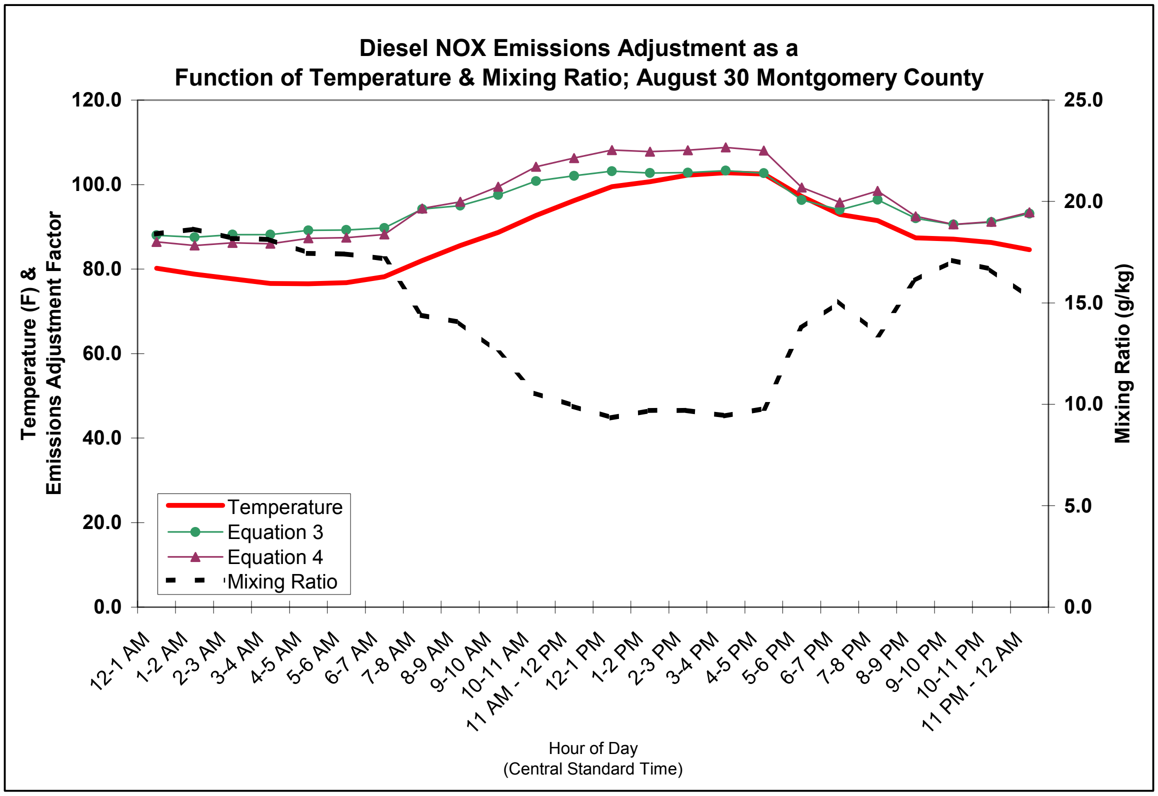


Figure 2-8. Diesel engine emissions adjustments for Montgomery County on August 30.

The NOx corrections for heavy-duty gasoline vehicles and equipment are typically much less important than the diesel correction because the NOx emission inventory for heavy-duty gasoline vehicles is usually about 10% of the diesel NOx emission inventory. Still the correction equation is different than that for diesel vehicles showing a greater reduction during low temperature evenings and early mornings and equivalent or higher adjustment factors during the higher temperature mid-day period. An example of the heavy-duty gasoline emission correction for Harris County is shown in Figure 2-9

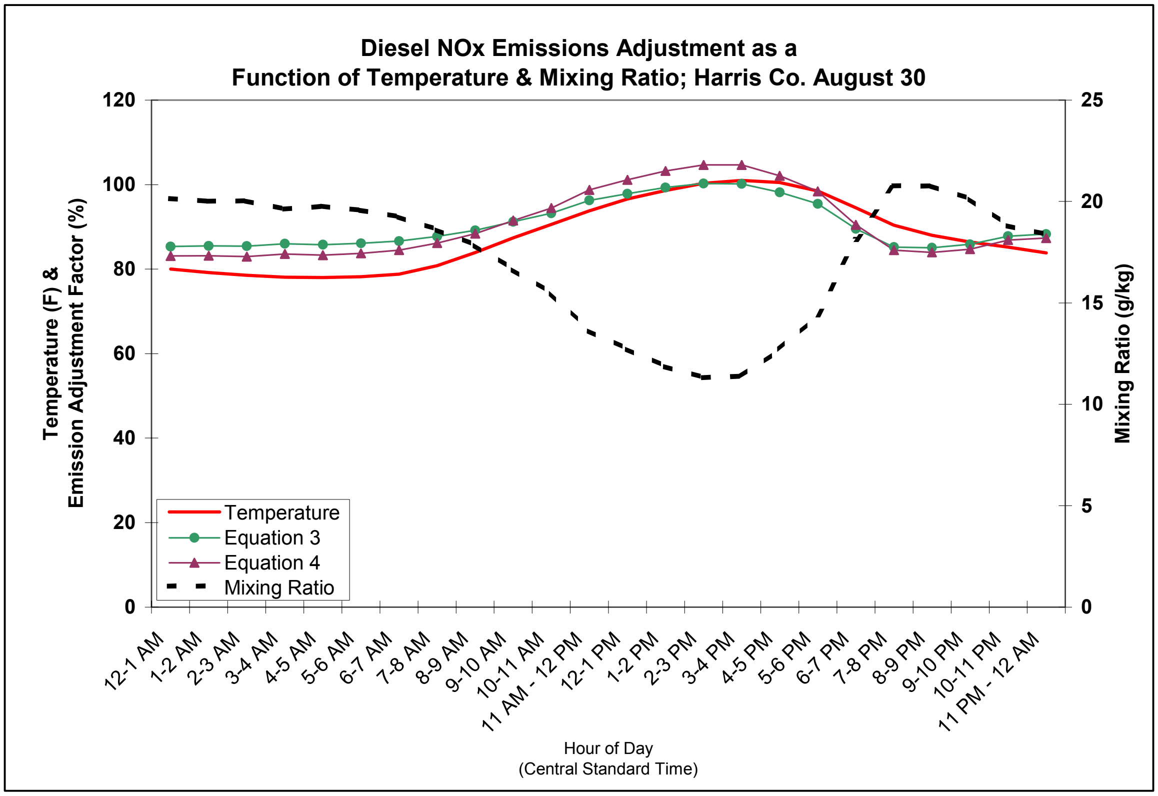


Figure 2-9. Gasoline engine emissions adjustments for Harris County on August 30.

Overall 24-hour county emission adjustments for the August 30 by county are shown in Table 2-1 and in Figure 2-10. The drier counties, such as Montgomery and Liberty, have much less adjustment compared with the coastal counties of Brazoria, Chambers, and Galveston reflecting the higher humidity near the Gulf. However, because Harris County dominates the emissions inventory, the emission adjustment primarily occurs in Harris County. The off-road results shown in Table 2-1 were performed with one set of ambient conditions for all eight counties, and so do not reflect the county-to-county effects as the on-road estimates do.

Table 2-1. NOx emission adjustment for on-road and off-road sources by county in 2007.

	Onroad August 30		Off-road August 31	
County	**NOx Adjustment (tpd)**	**NOx Adjustment (%)**	**NOx Adjustment (tpd)**	**NOx Adjustment (%)**
Brazoria	-0.5	-5.2 %	-0.5	-8.0 %
Chambers	-0.3	-7.5 %	Less than -0.1	-6.3 %
Fort Bend	-0.4	-2.7 %	-0.5	-8.1 %
Galveston	-0.9	-11.0 %	-0.3	-7.4 %
Harris	-5.3	-3.7 %	-2.9	-6.5 %
Liberty	0.02	0.6 %	-0.2	-8.8 %
Montgomery	-0.03	-0.2 %	-0.3	-8.1 %
Waller	-0.1	-2.6 %	-0.2	-8.8 %
8-County HGA Totals	**-7.4**	**-3.7 %**	**-4.8**	**-7.0 %**

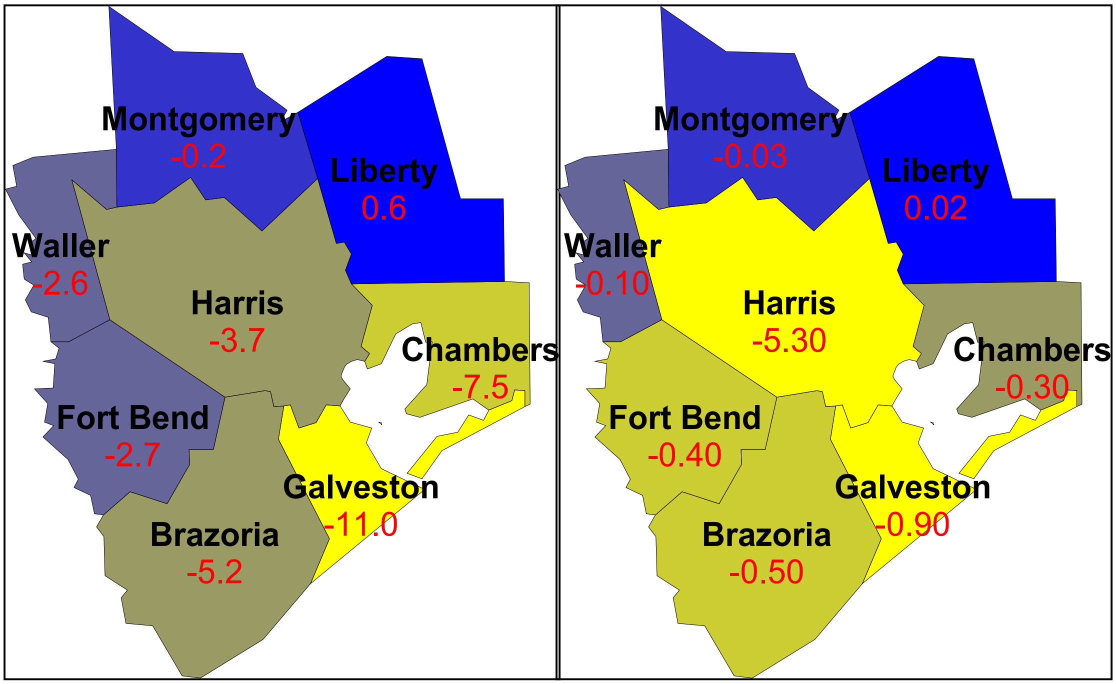


Figure 2-10. The NOx adjustment by county for August 30 for on-road vehicles in % (left) and tons per day (right).

The daily adjustments vary with the weather; so for the HGA episode the NOx adjustment ranged from a 0 to 10% reduction in the NOx emission inventory as shown in Table 2-2. The 8-county totals mostly reflect the adjustment of Harris County, which represents the overwhelming majority of 8-county emission totals. The relative adjustment (% effect) was calculated for the entire on-road inventory although the adjustment was applied only to the heavy-duty portion, so the correction to just the heavy-duty emission inventory is comparable (~6.4% on August 30 applied to 58% of the on-road emission inventory) to the off-road emission correction (~7 %).

Table 2-2. NOx emission adjustment for the on-road emission inventory in the 8-county area by episode day for 2007.

Day	On-road		Off-road	
	NOx Adjustment (tpd)	NOx Adjustment (%)	NOx Adjustment (tpd)	NOx Adjustment (%)
August 18	-6.0	-3.4 %	*-4.8*	*-7.0 %*
August 19	-5.5	-3.7	*-3.9*	*-6.6 %*
August 20	-2.6	-3.0	*-3.4*	*-6.8 %*
August 21	-10.3	-5.2	*-4.8*	*-7.1 %*
August 22	-15.4	-8.1	*-4.8*	*-7.1 %*
August 23	-15.3	-8.1	*-4.8*	*-7.1 %*
August 24	-16.3	-8.6	*-4.8*	*-7.0 %*
August 25	-9.3	-5.3	*-4.8*	*-7.0 %*
August 26	-7.5	-5.1	**-3.9**[1]	**-6.6 %**[1]
August 27	-3.0	-3.6	**-3.4**[1]	**-6.8 %**[1]
August 28	-11.0	-5.6	*-4.8*	*-7.1 %*
August 29	-11.1	-5.7	**-4.8**[1]	**-7.1 %**[1]
August 30	-7.4	-3.7	*-4.8*	*-7.1 %*
August 31	-1.9	-0.9	**-4.8**[1]	**-7.0 %**[1]
September 1	-5.6	-3.1	*-4.8*	*-7.0 %*
September 2	-6.0	-4.0	*-3.9*	*-6.6 %*

Day	On-road		Off-road	
	NOx Adjustment (tpd)	**NOx Adjustment (%)**	**NOx Adjustment (tpd)**	**NOx Adjustment (%)**
September 3	-1.0	-1.1	*-3.4*	*-6.8 %*
September 4	-0.4	-0.4	*-4.8*	*-7.1 %*
September 5	-3.2	-1.6	*-4.8*	*-7.1 %*
September 6	-5.8	-2.9	*-4.8*	*-7.1 %*

[1] These values used for Saturday – August 26, Sunday – August 27, Monday – Wednesday – August 29, Thursday & Friday – August 31.

The locomotive and marine adjustments are shown in Figures 2-11 and 2-12; for these results, 8-county average conditions were used. The primary difference between locomotive and marine adjustments was that the coastal stations would be used for the commercial marine adjustments, which have high and constant humidity levels typical of the marine environment. The higher humidity for marine conditions would result in lower NOx emissions than the inland adjustments would for locomotives.

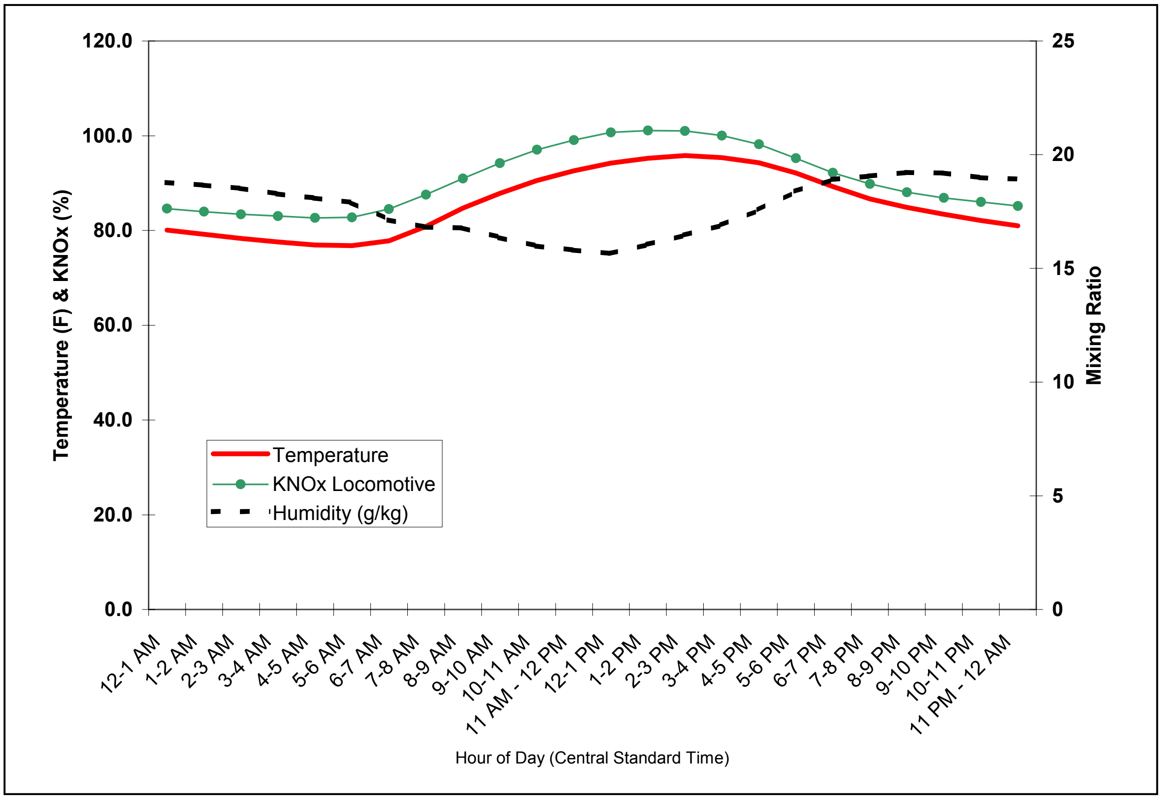


Figure 2-11. The NOx adjustment for locomotives for August 30.

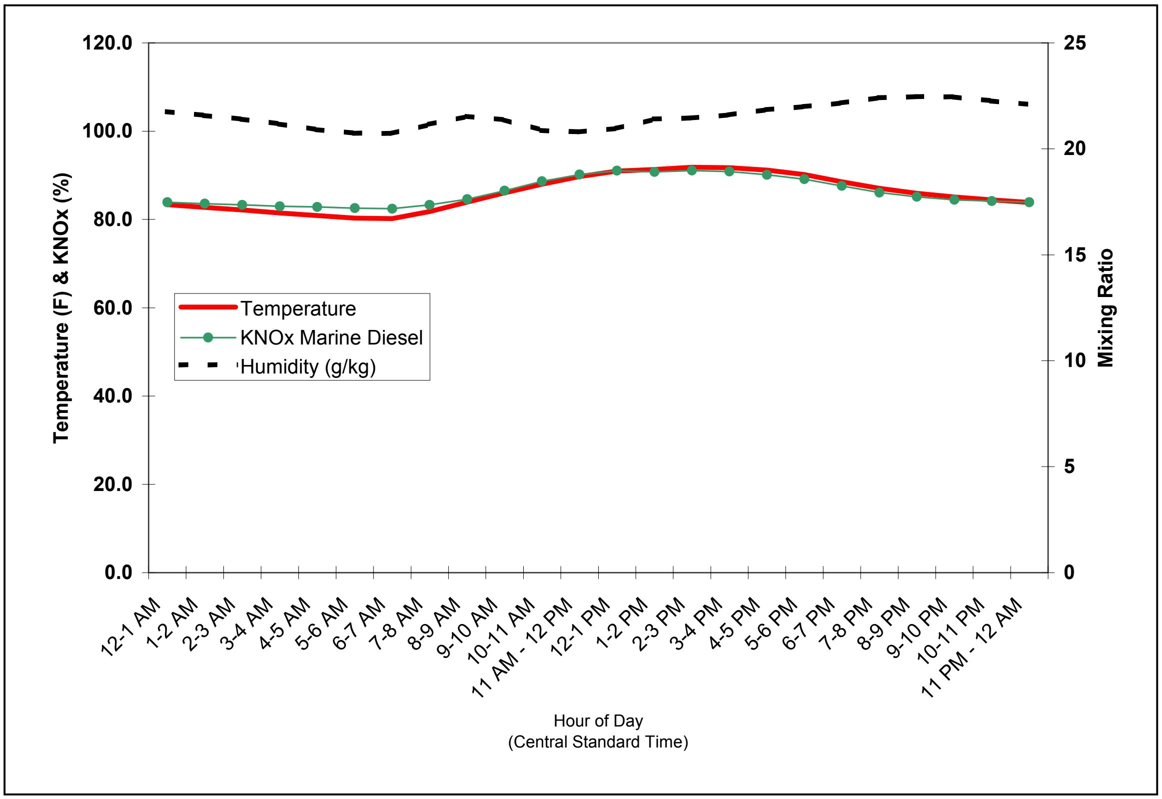


Figure 2-12. The NOx adjustment for commercial marine for August 30.

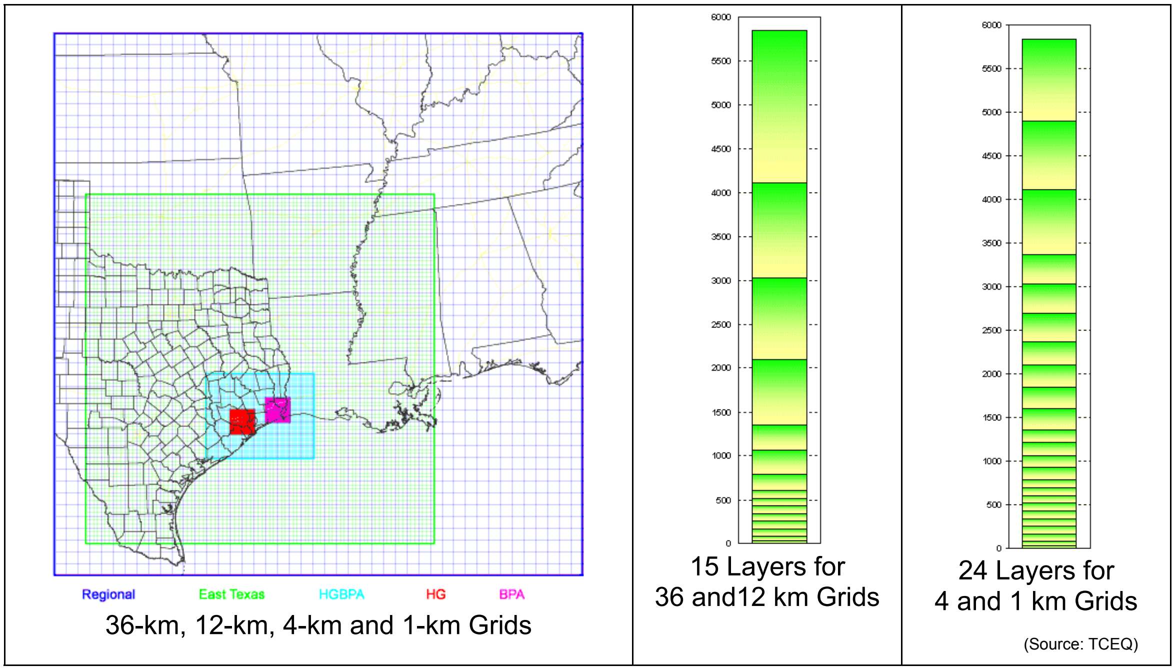
Overall the NOx adjustment for the humid HGA resulted in less than a 10% reduction in the 24-hour mobile source emissions inventory, but more significant NOx emission reductions occurred (~20%) during the early morning and late night conditions with either no reduction or slight increases in NOx emissions in the mid-day period. The effect of these adjustments on the ozone production and modeling performance is evaluated in Section 3. .

3. OZONE MODELING

This chapter describes the ozone modeling assessment of the impacts of correcting heavy-duty engine NOx emissions for humidity (the “NOx adjustment”). The evaluation used a modeling database developed by the TCEQ for current State Implementation Plan (SIP) modeling for the Houston/Galveston/Brazoria (HGB) and Beaumont/Port-Arthur (BPA) nonattainment areas (TCEQ 2004a). This HGBPA modeling database is described briefly below and in more detail in the TCEQ’s proposed mid-course review SIP for the HGB area (TCEQ, 2004b).

HOUSTON MODELING DATABASE

The HGBPA ozone modeling database was developed by the TCEQ for the period August 22 through September 6, 2000 which was during the Texas Air Quality Study (TexAQS). The CAMx modeling domain is shown in Figure 3-1.



36-km, 12-km, 4-km and 1-km Grids

15 Layers for 36 and12 km Grids

24 Layers for 4 and 1 km Grids

(Source: TCEQ)

Figure 3-1. CAMx nested grid modeling domain and layer structures for the TexAQS August 22 to September 6, 2000 episode period (Figures from TCEQ).

The TCEQ’s TexAQS modeling uses 2-way grid nesting. The outer (coarse) grid has 36-km spacing and a 12-km grid covers Eastern Texas, Louisiana and parts of neighboring states. The 36 and 12-km grids have 15 layers up to about 6 km and a 30 m surface layer. A 4-km grid covers the HG and BPA areas with enhanced vertical resolution of 24 layers. The extra vertical resolution in the 4-km grid adds layers between about 600 m and 6 km to better resolve the evolution of the mixing height and wind shears in the complex meteorological environment around the HGBPA. The TexAQS modeling domain also includes 1-km grids over HG and BPA. The 1-km grids were not used in this study because emissions data showing the impact of the NOx adjustment were not available at 1-km resolution. This is not considered a serious limitation in the modeling analysis because the spatial scale of the NOx adjustment is coarser than 1-km.

Data Sources

The main data sources for the modeling are summarized briefly below and are described in detail by TCEQ (2004b).

2000 Emissions: The emission inventories were prepared by the TCEQ in October 2004 and are referred to by their TCEQ version number of 5d (the elevated emissions were version 5c and the surface emissions were version 5d, so these are collectively referred to as 5d emissions). The TCEQ provided special emissions files for this study by preparing data files that included and excluded the NOx adjustment. The main data sources used by TCEQ in the version 5d inventories are listed in Table 3-1.

Table 3-1. Data sources used by TCEQ in preparing the HGBPA version 5d emission inventories for onshore sources.

Emissions Category	Data Source
On-road Mobile	EPA's MOBILE6 model with activity data from the Texas Department of Transportation (TxDOT) and the EPA
Off-road Mobile	EPA's NONROAD model version 2002
Point Sources	EPA's Acid Rain database for major utility sources; TCEQ's Point Source Database for 2000; Louisiana DEQ point source data; EPA's 1999 NEI for other States
Area Sources	TCEQ data for Texas EPA's 1999 NEI for States outside Texas
Off-shore emissions	Gulf of Mexico Air Quality Study (GMAQS) emission inventory grown from 1993 to 2000 by the TCEQ
Biogenics	GloBEIS Version 3.1

2007 Emissions: The TCEQ also provided 2007 future year emissions in October 2004 that are referred to by their TCEQ version number of cs08 (the elevated emissions were version cs06b and the surface emissions were version cs08, so these are collectively referred to as cs08 emissions). The 2007 emissions were projected from the 2000 emissions to account for growth in activity levels and the effects of emission control strategies in the Houston area and throughout the modeling domain (TCEQ, 2004b).

Meteorology: The meteorological input data were prepared using the PSU/NCAR Mesoscale Model, version 5 (MM5). The MM5 simulations for August 22 through September 1, 2000 were completed by Texas A&M University (Nielsen-Gammon, 2003) whereas the MM5 simulations for September 2 through 6, 2000 were completed by Atmet/ENVIRON (Atmet, 2003). Two separate MM5 simulations were performed because the period September 2 through 6 was an extension to the original modeling period. MM5 data were formatted for CAMx by the TCEQ using ENVIRON's MM5CAMx preprocessor.

Initial and Boundary Conditions: The initial conditions and boundary conditions (IC/BCs) were developed by TCEQ following the procedures developed by ENVIRON for an earlier regional modeling study (Yocke et al., 1996). The BCs varied by geographic region to provide clean air BCs out over the Gulf and emissions influenced BCs over land. The difference between the West and East/Northeast boundary segments is to represent the impact of biogenic VOC emissions in the Southeastern U.S. (Goldan, Kuster, and Fehsenfeld; 1995). The boundary conditions for 2007 were assumed to be the same as for 2000 (TCEQ, 2004b).

Model Version and Options

The modeling analyses used version 4.03 of CAMx (ENVIRON, 2004). The CAMx model options selected by TCEQ were:

- Piecewise parabolic method (PPM) advection scheme (Colella and Woodward, 1984). This is the numerical method used for horizontal advection and PPM is selected because it is less numerical diffusion than older schemes such as the Smolarkiewicz (1983) scheme used in the UAM-IV.

- Carbon Bond 4 (CB4) chemistry (Gery et al., 1989) with updates to PAN chemistry, isoprene chemistry and radical-radical reactions (ENVIRON, 2004). This version of CB4 was developed for the Ozone Transport Assessment Group (OTAG) modeling.

- Dry deposition was selected. CAMx uses the Wesely (1989) algorithm developed for the Regional Acid Deposition Model (RADM) with updates described in the User's Guide (ENVIRON, 2004).

- Wet deposition was selected. The CAMx wet deposition scheme is based on Seinfeld and Pandis (1998) and is described in the User's Guide (ENVIRON, 2004).

- The CAMx plume-in-grid (PiG) algorithm (ENVIRON, 2004) was selected for major NOx point sources. The PiG accounts for the near source dispersion and chemistry of NOx emissions from major sources before the source plumes are large enough to be resolved by the CAMx grids.

OBSERVED AND MODELED OZONE LEVELS

The TCEQ evaluated the performance of the Houston modeling system in detail (TCEQ, 2004c) Short summaries of the TexAQS episode conditions and the TCEQ performance evaluation are included here to provide context for the model sensitivity results that follow.

Observed Ozone Levels and Meteorology During the TexAQS Episode

The August 16-September 6, 2000 ozone episode occurred during the peak of the ozone season and included a full suite of daily wind directions, indicative of a full synoptic cycle. In addition, days with persistent land breezes and days with stagnation/flow reversal are present. The period 3was characterized by 13 one-hour ozone exceedances and 14 eight-hour ozone exceedances. For these reasons, the episode is considered by TCEQ staff as fully representative of typical ozone patterns in the Houston area. Observed ozone levels and meteorology for the episode is discussed in detail in the modeling protocol development by the TCEQ (TCEQ, 2004a). The period August 22- September 6, being modeling for this study, can be summarized as follows:

- Beginning on August 22, a period of relatively low ozone lasting until August 25 was experienced. On August 25, 12 monitors recorded one-hour exceedances, while 9 monitors recorded eight-hour exceedances. August 25 was characterized by a fairly compact parcel of westward moving ozone-laden air which brought very high ozone levels to some areas; the 1-hour peak was 194 ppb. The 8-hour peak was 111 ppb.

- August 26 saw relatively modest exceedances of both the one- and eight-hour standard (140 and 94 ppb, respectively), both of which occurred north of the urban core in Conroe.

- August 27 and 28 saw relatively low ozone concentrations (although the eight-hour peak on August 28 was just below the standard at 84 ppb). Beginning on August 29, both the one- and eight-hour standards were exceeded for nine consecutive days.

- On August 29, four monitors recorded eight-hour exceedances while three recorded exceedances of the one-hour standard. Peak eight-hour ozone was 99 ppb, while the one-hour peak was 146 ppb.

- On August 30, the highest one-hour concentration of the entire year was recorded; 199 ppb at the HRM-8 monitor in LaPorte. The eight-hour peak was also very high, 144 ppb. Despite its intensity, the area of high ozone was not especially large, with six monitors exceeding the eight-hour standard and seven exceeding the one-hour standard.

- The following day, August 31 saw more widespread ozone with sixteen monitors recording eight-hour peaks over 85 ppb and 10 recording one-hour concentrations above 125 ppb. Despite the broad area affected, peak one- and eight-hour concentrations, 168 and 130 ppb, respectively, were significantly lower than on the previous day.

- On September 1, one-hour exceedances were recorded at only two monitors, and eight-hour exceedances at three monitors, as the winds transported much of the city's pollution eastward. The one-hour peak was still fairly large at 163 ppb, although the eight-hour peak was a relatively moderate 102 ppb.

- September 2 and 3 had minimal one-hour exceedances, 125 and 127 ppb, respectively, at a single station on each day. Eight-hour exceedances, however, were more widespread with eight and four stations, respectively, exceeding the 8-hour standard. Peak 8-hour ozone on September 2 was 95 ppb, followed by 93 ppb on September 3.

- On September 4, three monitors exceeded the 8-hour standard with a peak of 90 ppb. One-hour ozone was higher, peaking at 145 ppb at one of the two monitors recording exceedances on that day.

- On September 5, a peak 1-hour ozone concentration of 185 ppb was recorded, although only three monitors reported one-hour exceedances. Nine monitors, however, reported 8-hour ozone exceedances with a peak of 120 ppb.

- September 6 also recorded a relatively high one-hour peak of 156 ppb at the only station exceeding the 1-hour standard. Again, the eight-hour exceedance area was fairly widespread with six monitors reporting exceedances with a peak of 123 ppb.

Table 3-2 provides a summary of the observed ozone levels and meteorology during the episode.

Table 3-2. Summary of the August 22 – September 6, 2000 HGB ozone episode.

Episode Day	Measured Sfc Max Ozone	Peak Station	# Sfc Stations Exceeding	Aircraft Measured Ozone	Flow Reversal?
August 22	107 ppb	Aldine	0	80 ppb	Yes
August 23	101 ppb	Bayland Park	0	149 ppb	Yes
August 24	120 ppb	La Porte	0	128 ppb	Yes
August 25	194 ppb	Crawford	12	233 ppb	Yes*
August 26	140 ppb	Conroe	1	152 ppb	Yes
August 27	87 ppb	Conroe	0	115 ppb	Sea Breeze
August 28	112 ppb	Conroe	0	140 ppb	Sea Breeze
August 29	146 ppb	Mt Belview	3	211 ppb	Yes
August 30	200 ppb	La Porte	7	220 ppb	Yes
August 31	175 ppb	La Porte	10	194 ppb	Yes
September 1	163 ppb	E Baytown	2	210 ppb	Land Breeze
Sept 2	125 ppb	Deer Park	1		Sea Breeze
Sept 3	127 ppb	E Baytown	1	153 ppb	Sea Breeze
Sept 4	164 ppb	Texas City	2	132 ppb	Yes
Sept 5	185 ppb	Galveston	3	239 ppb	Land Breeze
Sept 6	156 ppb	Croquet	1	160 ppb	Land Breeze
Totals	13 Exc Days	---	53 Exc Sites	17 Exc Days	

TexAQS 2000 Episode Ozone Model Performance

The TCEQ evaluated the performance of the Houston ozone modeling system with base 5b emissions and including a 1-km grid over the Houston area (Figure 3-1). Table 3-3 summarizes the statistical model performance measures for one-hour ozone (defined in Table 3-4) and Figure 3-3 (from TCEQ, 2004c) illustrates the model performance for 8-hour ozone. The complete TCEQ evaluation of base case model performance is presented in TCEQ (2004c).

Table 3-3. Model performance evaluation with base 5b emissions and 1-km Houston grid reported by TCEQ (2004c).

	For observations above 60 ppb		Area-wide peak ozone		
Episode Date	**Normalized Bias ±(5-15)%**	**Normalized Gross Error (30-35)%**	**Accuracy ±(15-20)%**	**Modeled Peak ppb**	**Observed Peak ppb**
8/22/2000	-37.7	39.3	0.2	107.3	107.0
8/23/2000	-48.9	48.9	-18.4	82.4	101.0
8/24/2000	-38.5	38.5	-34.8	78.4	120.1
8/25/2000	-9.9	20.9	-19.3	156.5	194.0
8/26/2000	6.3	18.5	6.7	149.4	140.0
8/27/2000	25.2	25.2	29.0	112.3	87.0
8/28/2000	22.4	24.3	17.8	132.0	112.0
8/29/2000	8.1	15.8	3.1	151.2	146.7
8/30/2000	-11.0	20.4	-31.6	137.2	200.5
8/31/2000	4.6	15.8	-1.4	173.0	175.5
9/1/2000	8.1	13.7	-16.5	136.7	163.7
9/2/2000	-2.7	17.1	21.7	152.7	125.5
9/3/2000	-3.1	19.6	10.2	140.1	127.2
9/4/2000	5.7	20.4	9.0	158.1	145.0
9/5/2000	7.0	26.6	13.4	209.9	185.0
9/6/2000	-5.1	18.9	-2.0	152.9	156.0

Note:

Yellow-shaded cells are outside the EPA performance goal (shown in column heading).

Table 3-4. Statistical measures for air quality model performance evaluation.

Statistical Measure	Mathematical Expression	Notes
Accuracy of unpaired peak	$\frac{P_{peak} - O_{peak}}{O_{peak}}$	EPA Goal for 1-hour ozone of less than ±(15-20)% P_{peak} over all grid cells O_{peak} over all monitors
Average paired peak accuracy	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left(P_{peak} - O_{peak}\right)}{O_{peak}}$	No EPA Goal for 1-hour ozone P_{peak} and O_{peak} are paired in space but not time at each monitor
Normalized Gross Error	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left\|P_i - O_i\right\|}{O_i}$	EPA Goal for 1-hour ozone of less than 30-35% P_i and O_i are paired values over all monitors when $O_i \geq 60$ ppb
Normalized Bias	$\frac{1}{N}\sum_{i=1}^{N}\frac{\left(P_i - O_i\right)}{O_i}$	EPA Goal for 1-hour ozone of less than ±(5-15)% P_i and O_i are paired values over all monitors when $O_i \geq 60$ ppb

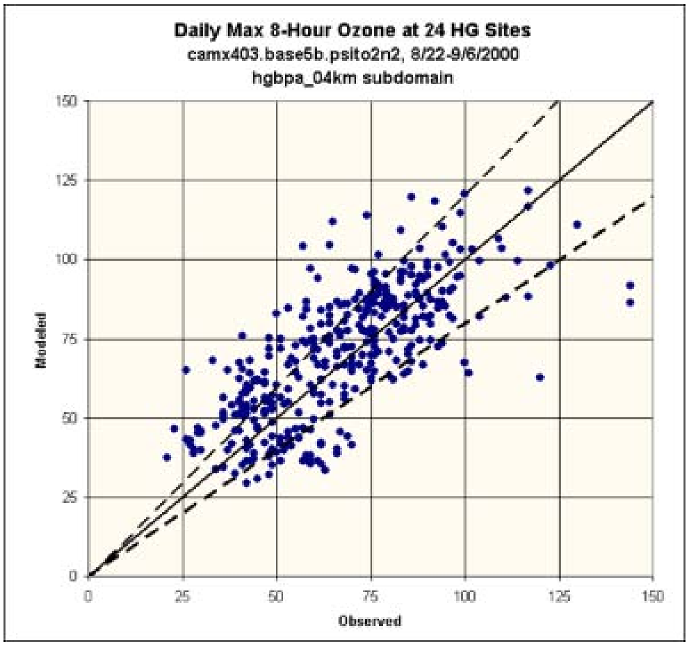


Figure 3-2. Daily modeled eight-hour peak ozone vs. observed peaks at 24 sites in the Houston-Galveston area (from TCEQ, 2004c).

IMPACT OF THE NOx ADJUSTMENT ON MODELED OZONE LEVELS

Four model runs were completed to determine the impact of the NOx adjustment in 2000 and 2007:

1 2000 NOx adjustment (base 5d emissions)
2 2000 No NOx adjustment
3 2007 NOx adjustment (cs08 emissions)
4 2007 No NOx adjustment

The impact of the NOx adjustment in year 2000 is the difference between the first two runs and the impact for 2007 is the difference between the last two model runs. The only differences between runs were the presence/absence of the NOx adjustment in the emission inventories. Because the TCEQ includes the NOx adjustment in Houston modeling inventories the runs with the NOx adjustment are the 2000 base 5d and 2007 cs08 scenarios.

Impact on Ozone Levels in 2000 and 2007

Daily maximum 1-hr ozone levels in the 4-km grid covering the HGBPA area are shown in Figures 3-3 to 3-5 for August 25th and 30th and September 5th. In these Figures, the left column is for 2000 and the right column for 2007, the top row includes the NOx adjustment, the middle row has no NOx adjustment and the bottom row is the difference (with - without the NOx adjustment). Table 3-5 shows the largest increases and decreases in daily maximum 1-hour ozone (with - without the NOx adjustment) in the HGBPA 4-km grid for each modeling day. The three days shown in Figures 3-3 to 3-5 showed the largest impact of the NOx adjustment (see Table 3-5) and also were the days with highest observed 1-hour ozone levels (see Table 3-3).

The NOx adjustment reduced NOx emissions in the Houston area (see Chapter 2) and the largest NOx decreases (in tons/day) were in Harris County (see Figure 2-5). The amount of NOx decrease varies with time of day and reductions occur predominantly at night and in the early morning. This means that there generally is less NOx available at the start of each day with the NOx adjustment.

The NOx adjustment causes both increases and decreases in maximum 1-hour ozone levels for year 2000 (Table 3-5). In general, ozone decreases resulting from a NOx decrease indicate NOx-limited ozone formation, whereas ozone increases from a NOx decrease indicate VOC-limited ozone formation. The ozone difference plots in Figures 3-3 to 3-5 show that ozone increases/decreases occur in different geographic locations depending upon the day and the year (2000 vs. 2007). For year 2000 on August 25th and 30th the areas of high 1-hour ozone show ozone increases due to the NOx adjustment, whereas on September 5th the area of high 1-hour ozone shows ozone decreases due to the NOx adjustment. The modeling results for year 2000 show that ozone formation in the Houston modeling cannot be categorized simply as NOx-limited or VOC-limited across all episode days, and so the impact of the NOx adjustment varies with day and location.

The 2007 ozone modeling shows both increases and decreases in maximum 1-hour ozone levels due to the NOx adjustment, as for 2000. Table 3-5 shows smaller increases in daily maximum ozone in 2007 than 2000 indicating a shift toward more NOx-limited conditions in 2007 relative to 2000. This is confirmed by the ozone difference plots for August 25th and 30th (Figures 3-3 and 3-4) that show large reductions in the area of ozone increases in 2007 compared to 2000. The balance between NOx-limited and VOC-limited conditions is expected to shift toward NOx-limited conditions in 2007 because of reductions in NOx emission levels. The largest decreases in ozone (Table 3-5) are smaller in 2007 than 2000 because the NOx emission reductions were smaller in magnitude (i.e., tons/day) in 2007 than 2000.

Table 3-5. Largest differences (with - without the NOx adjustment) in daily maximum 1-hour ozone in the 4-km grid for each modeling day in 2000 and 2007.

	Ozone Difference (ppb) due to the NOx adjustment			
	2000		2007	
Day	Min	Max	Min	Max
August 22	-1.0	4.5	-0.9	1.8
August 23	-1.2	4.1	-1.1	2.0
August 24	-0.9	2.6	-0.8	1.1
August 25	-1.3	6.4	-1.0	1.2
August 26	-0.6	2.3	-0.9	1.0
August 27	-0.6	0.2	-0.5	0.1
August 28	-1.6	1.1	-1.1	0.1
August 29	-1.2	3.0	-0.9	0.5
August 30	-1.1	7.8	-1.0	1.3
August 31	-1.1	3.2	-0.8	0.7
September 1	-1.3	1.9	-1.0	0.3
September 2	-0.9	0.2	-0.8	0.0
September 3	-0.5	0.2	-0.4	0.2
September 4	-0.6	0.1	-0.4	0.1
September 5	-2.3	1.6	-1.4	0.7
September 6	-0.4	0.4	-0.6	0.3

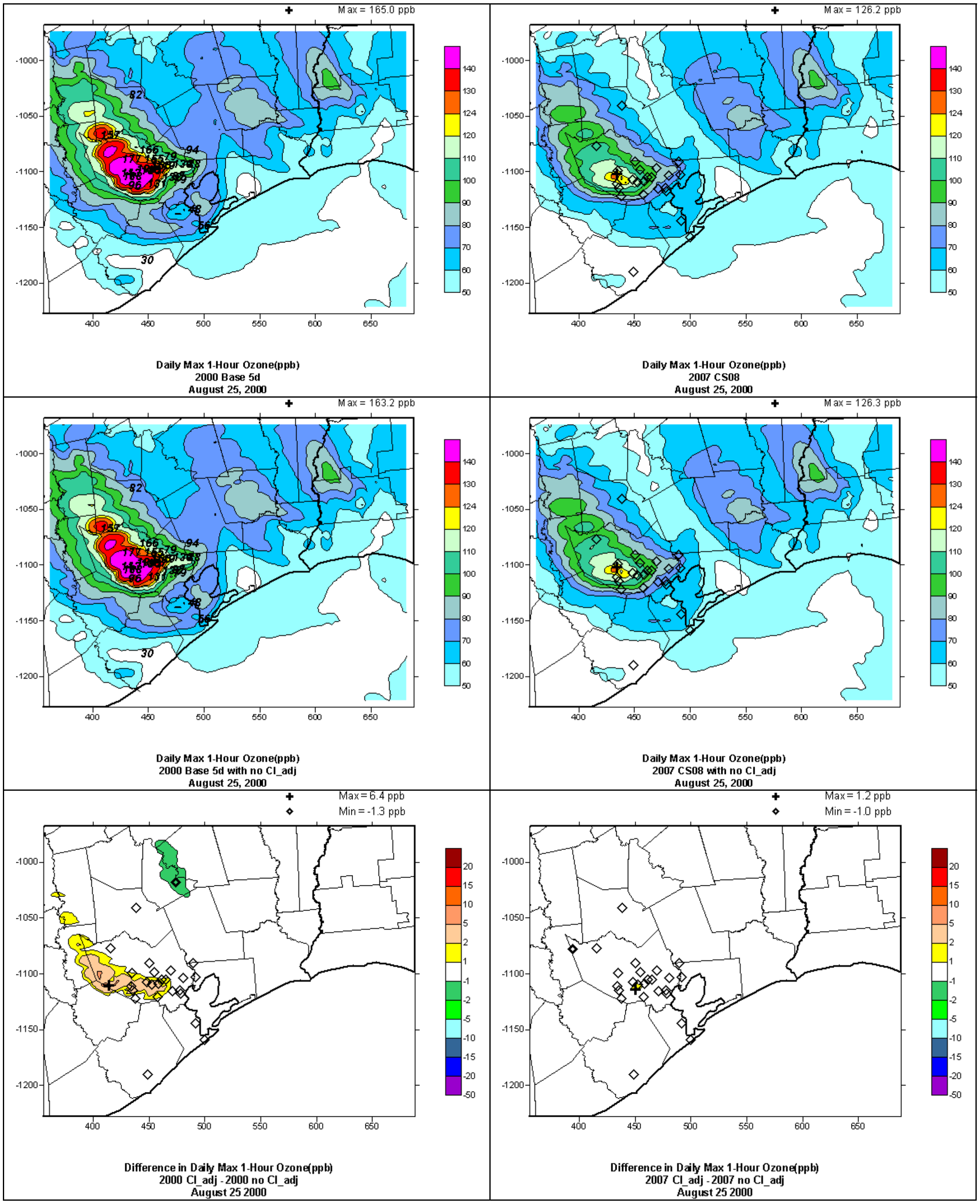
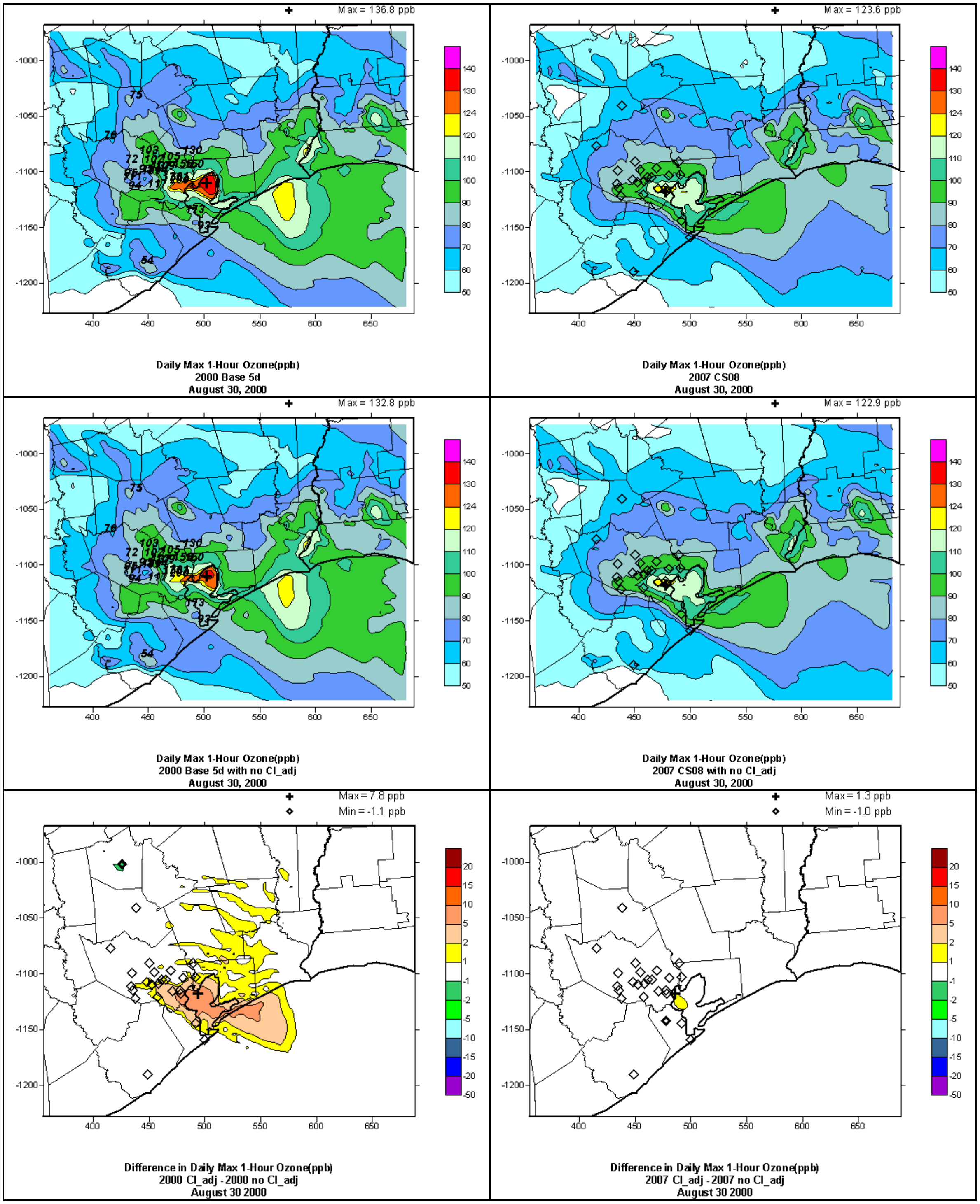


Figure 3-3. Impact of the NOx adjustment on daily maximum 1-hour ozone in the 4-km grid on August 25th for: Year 2000 (left) and 2007 (right).



Daily Max 1-Hour Ozone(ppb)
2000 Base 5d
August 30, 2000

Daily Max 1-Hour Ozone(ppb)
2007 CS08
August 30, 2000

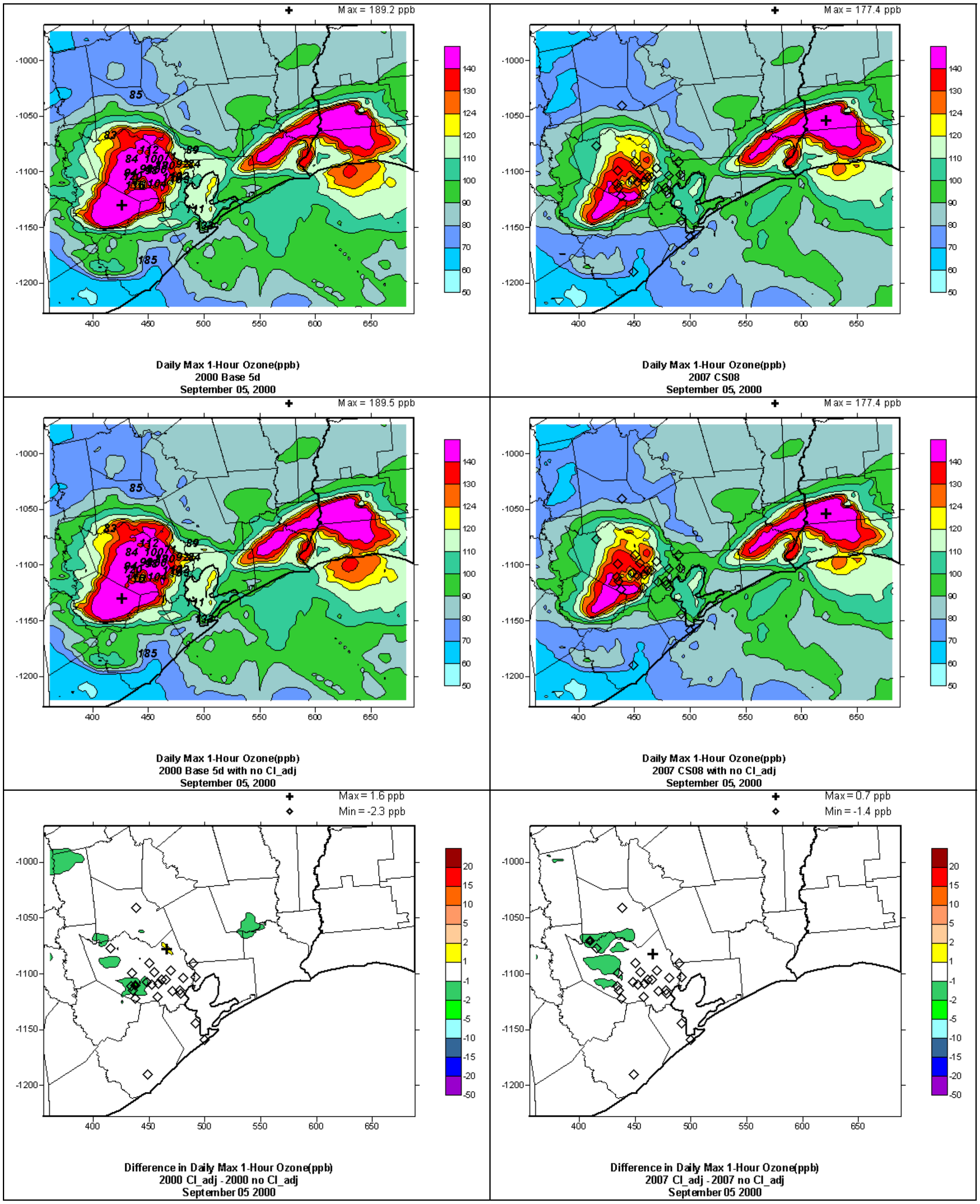
Daily Max 1-Hour Ozone(ppb)
2000 Base 5d with no Cl_adj
August 30, 2000

Daily Max 1-Hour Ozone(ppb)
2007 CS08 with no Cl_adj
August 30, 2000

Difference in Daily Max 1-Hour Ozone(ppb)
2000 Cl_adj - 2000 no Cl_adj
August 30 2000

Difference in Daily Max 1-Hour Ozone(ppb)
2007 Cl_adj - 2007 no Cl_adj
August 30 2000

Figure 3-4. Impact of the NOx adjustment on daily maximum 1-hour ozone in the 4-km grid on August 30th for: Year 2000 (left) and 2007 (right).



Max = 189.2 ppb

Daily Max 1-Hour Ozone(ppb)
2000 Base 5d
September 05, 2000

Max = 177.4 ppb

Daily Max 1-Hour Ozone(ppb)
2007 CS08
September 05, 2000

Max = 189.5 ppb

Daily Max 1-Hour Ozone(ppb)
2000 Base 5d with no Cl_adj
September 05, 2000

Max = 177.4 ppb

Daily Max 1-Hour Ozone(ppb)
2007 CS08 with no Cl_adj
September 05, 2000

Max = 1.6 ppb
Min = -2.3 ppb

Difference in Daily Max 1-Hour Ozone(ppb)
2000 Cl_adj - 2000 no Cl_adj
September 05 2000

Max = 0.7 ppb
Min = -1.4 ppb

Difference in Daily Max 1-Hour Ozone(ppb)
2007 Cl_adj - 2007 no Cl_adj
September 05 2000

Figure 3-5. Impact of the NOx adjustment on daily maximum 1-hour ozone in the 4-km grid on September 5th for: Year 2000 (left) and 2007 (right).

Impact on Model Performance for Year 2000

The impact of the NOx adjustment on ozone levels for year 2000 was discussed above. Statistical measures of model performance (defined in Table 3-4) were calculated for the 2000 simulations with and without the NOx adjustment and are compared in Figure 3-6. Time series of predicted and observed ozone at several monitors in the Houston area (Figure 3-7) are compared in Figure 3-8. The effects of the NOx adjustment on both the ozone time series and model performance statistics were small and cannot be used to decide whether the NOx adjustment is "correct" or not.

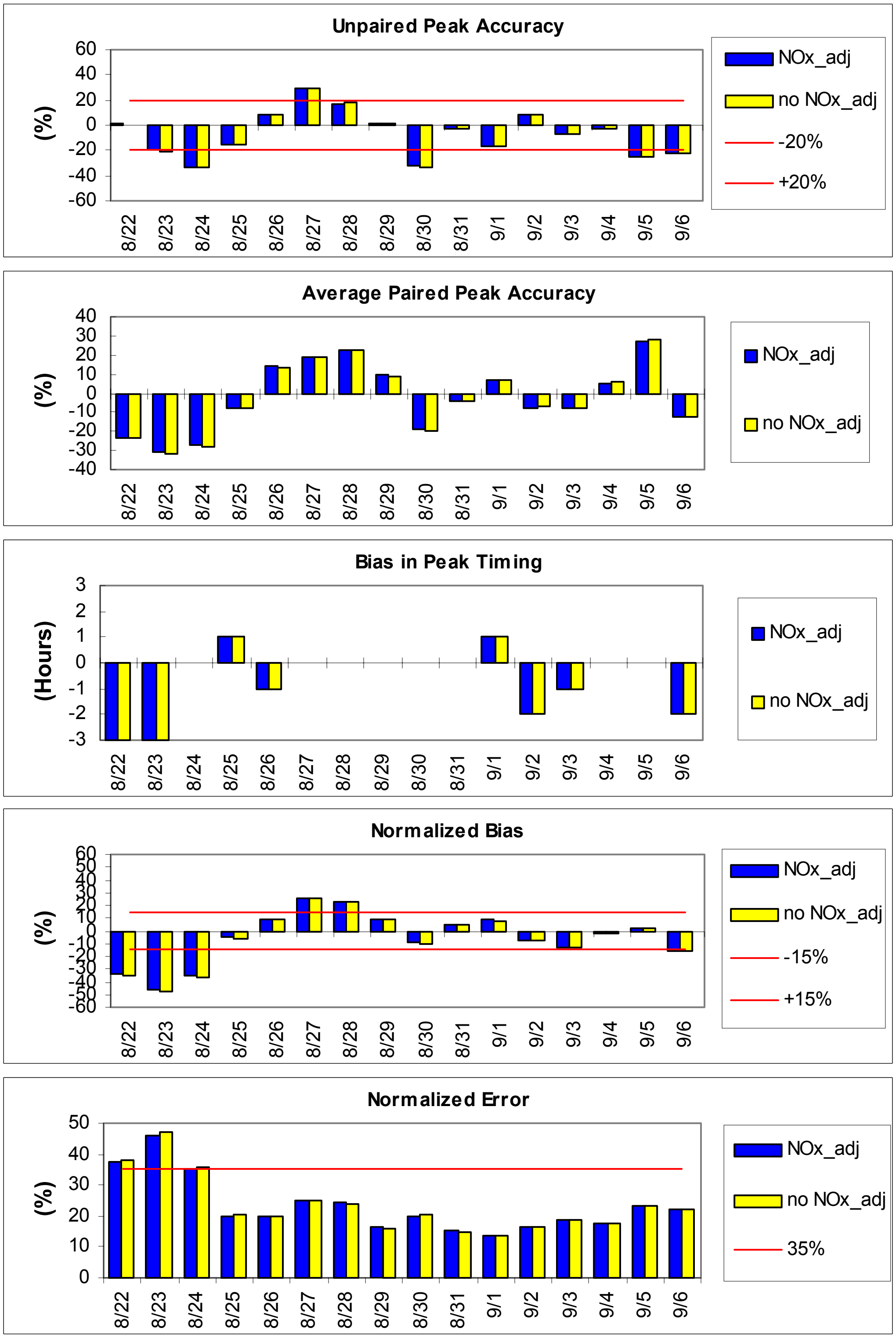


Figure 3-6. Impact of the NOx adjustment on model performance with base 5d emissions and without a 1-km Houston grid.

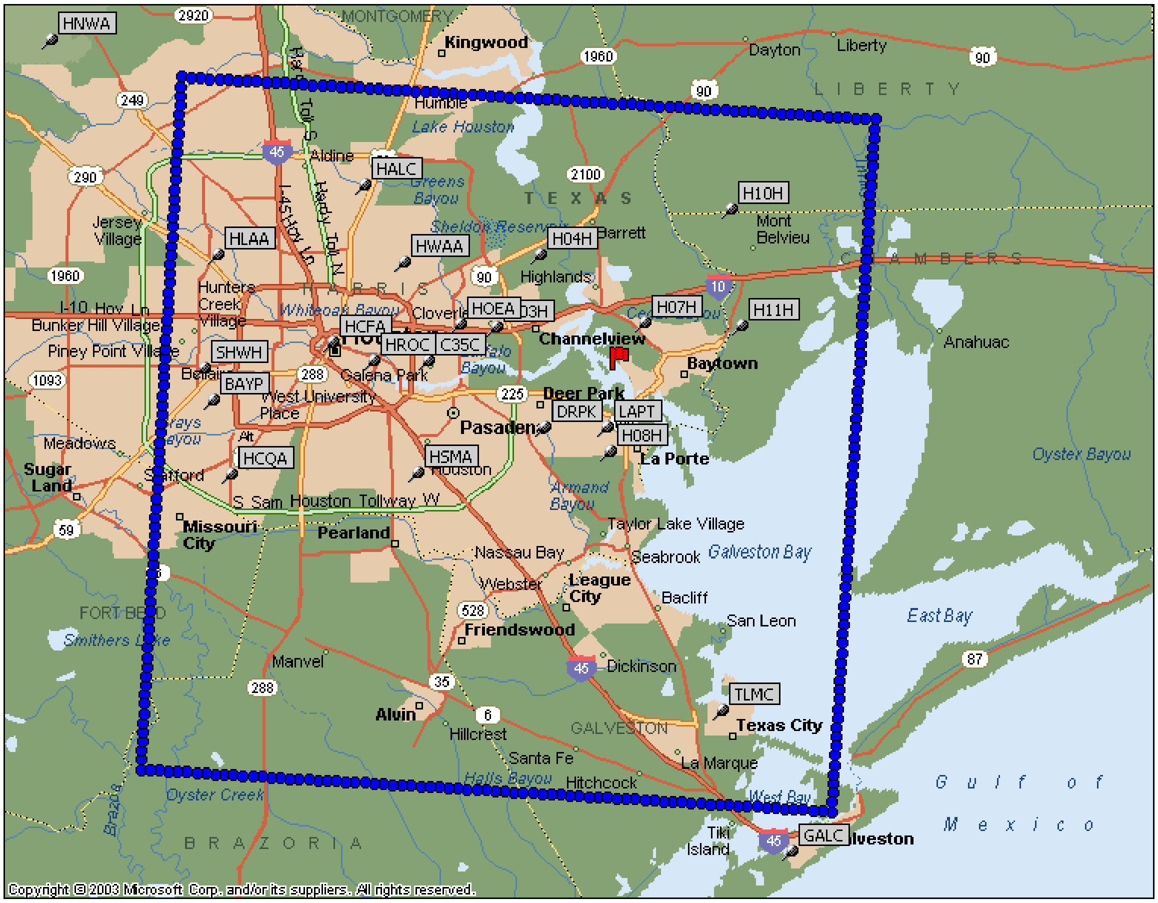


Figure 3-7. Location of ozone monitors in the Houston area and the boundary of the 1-km grid used by TCEQ (in blue).

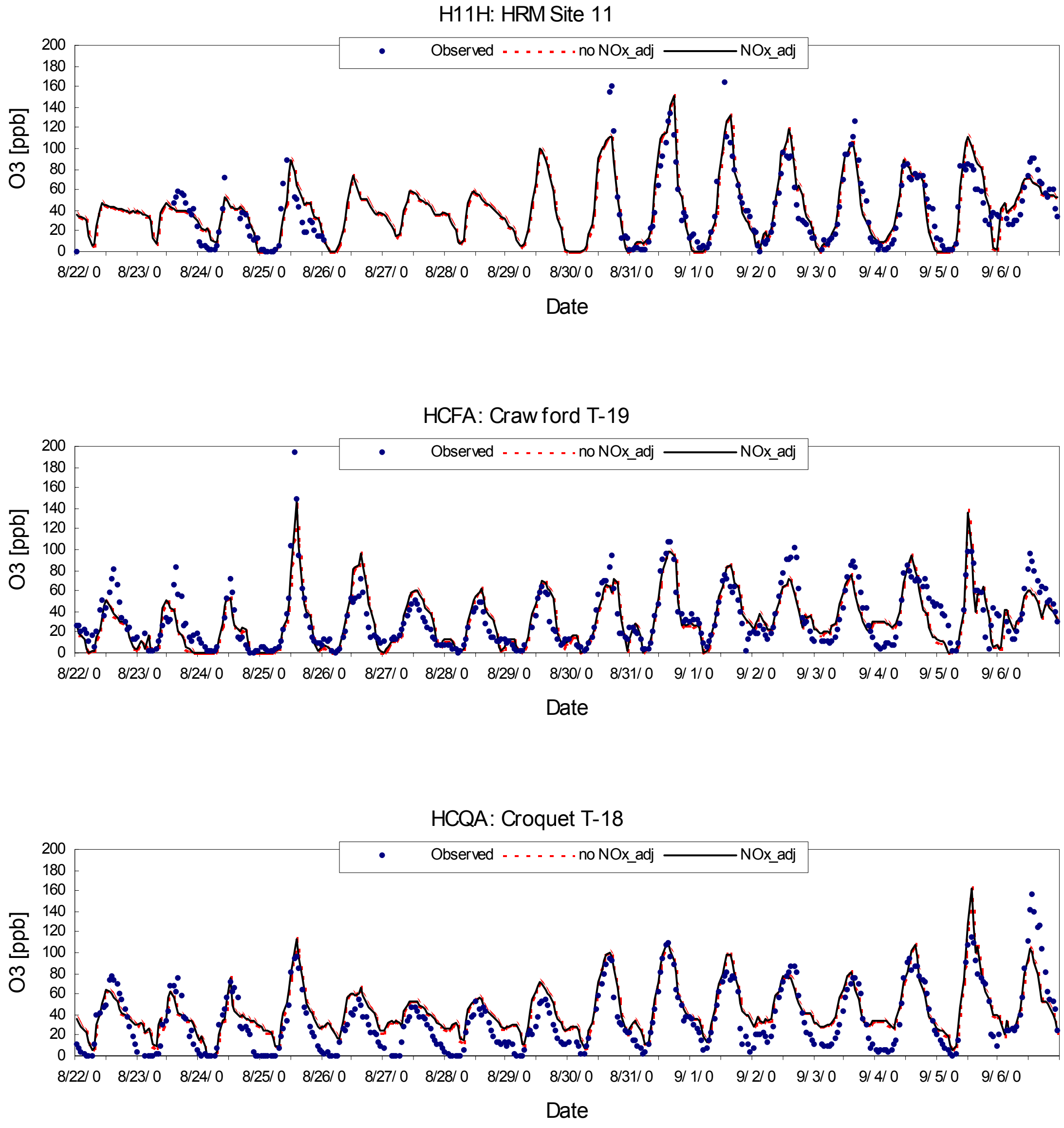


Figure 3-8. Impact of the NOx adjustment on time series for several ozone monitors in the Houston area. (Part 1)

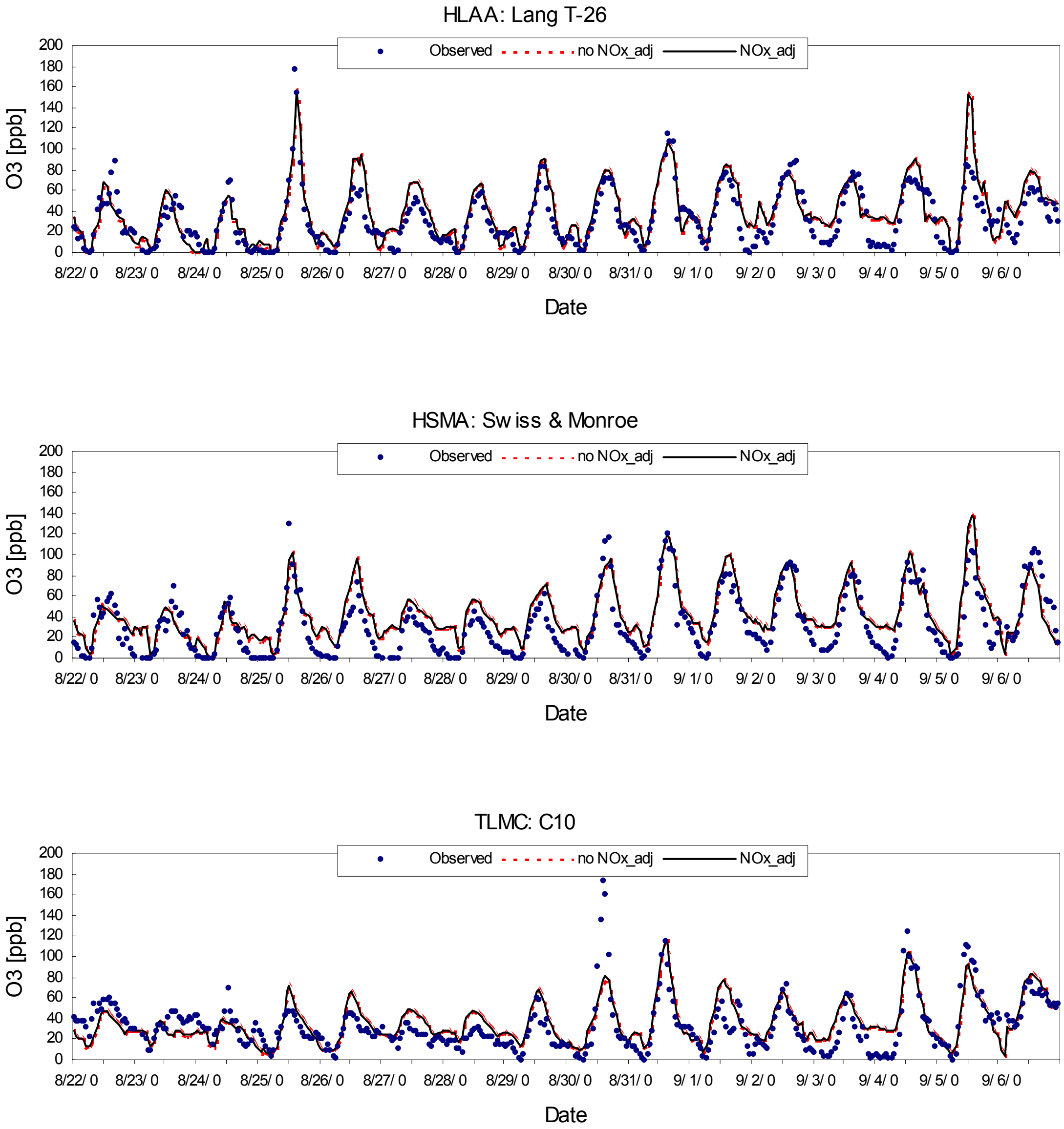


Figure 3-8. (concluded). Impact of the NOx adjustment on time series for several ozone monitors in the Houston area.

4. CONCLUSIONS

Texas has led the way in improved air quality evaluation and modeling by developing several innovative techniques and evaluations. One of the more important considerations is to accurately estimate emissions temporally and spatially. This is important not just to improve the predicted air quality but also to focus control strategies on the most effective and cost-effective emission sources. Heavy-duty vehicles and off-road equipment have become increasingly important emission sources categories because light-duty vehicles and stationary source emissions have experienced more control efforts. This work developed methods to incorporate ambient humidity and temperature effects (spatially and temporally) on the estimated NOx emissions from on-road heavy-duty vehicles and off-road engines for the Houston-Galveston nonattainment area (HGA).

The conclusion reached in this work is that humidity and temperature corrections to the NOx emissions rates from internal combustion engines should be included in the modeled emission inventory. ENVIRON provided TCEQ as part of this work a new software tool called CNTRLHR to use in adjusting the modeled emission inventory by hour of day. The adjustment described in this work did not significantly change ozone model performance for the year 2000 base case for HGA. The effects of the adjustment on future year 2007 modeled ozone levels were less than modeled for 2000 because the baseline mobile source NOx emissions are less in 2007.

The effect of ambient humidity and temperature corrections has been included in all reported emission measurements used in developing emission models and estimates. The historical data and scientific understanding indicates that higher humidity results resulting in lower NOx emissions from internal combustion engines used in on-road vehicles and off-road equipment, and higher temperature increases NOx emissions from engines without aftertreatment devices and after those with aftertreatment devices have reached their operating temperature. Except for light-duty on-road vehicle emissions estimates, EPA has not included these ambient condition adjustments to NOx emission rates of on-road heavy-duty vehicles and off-road equipment.

The NOx adjustments for the ambient conditions were applied to the emission inventory of the HGA for on-road heavy-duty and off-road equipment. Because the modeling in this work was performed for a relatively humid area, overall NOx emission decreases were predicted, more significant decreases in night and early morning and less significant decreases and some increases in midday. Though HGA is a region generally considered very humid, the NOx emission reductions were less than 10% of affected sources, and the overall change emissions was less significant when considering all sources in the region. A drier region that reaches similar or higher daily temperature may be predicted to have higher NOx emissions than models currently predict.

The results of the CAMx ozone modeling for HGA revealed several conclusions for the base year case of 2000 and the future attainment year of 2007. The ambient humidity and temperature adjustments caused both increases and decreases in maximum 1-hour ozone levels for year 2000 depending upon day and location. Ozone increases occurred in areas where ozone levels were VOC-limited. The adjustment did not significantly change ozone model performance for the year 2000 base case. Because the effect of the adjustments on model performance was small the ozone modeling should no be used to decide whether or not the adjustment is “correct”.

The 2007 ozone modeling shows both increases and decreases in maximum 1-hour ozone levels due to the NOx adjustment, as for 2000. The increases in daily maximum ozone in 2007 were smaller than in 2000, indicating a shift toward more NOx-limited conditions in 2007 relative to 2000.

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APPENDIX A

Southwest Research Institute Report:
"Humidity and Temperature Correction Factors For NO_x Emissions From Diesel Engines"

HUMIDITY AND TEMPERATURE CORRECTION FACTORS FOR NO_X EMISSIONS FROM DIESEL ENGINES

FINAL REPORT

SwRI Project No. 03.30.10.06599

Prepared for:

ENVIRON International Corporation
101 Rowland Way, Suite 220
Novato, CA 94945-5010

June 2003

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1.0 BACKGROUND

Emission regulations continue to place additional restrictions on urban areas trying to achieve ambient air quality standards. Although ambient air quality standards are national, achieving the standards is a regional problem delegated to the states. However, the certification procedures for diesel engines are standardized without regard for regional variation in ambient conditions like temperature and humidity. As early as 1970(1), it was recognized that engine NO_x emissions are significantly affected by the thermodynamic conditions of the intake air. Specifically, the intake air temperature and humidity have the dominant effects(1-3). Because of these sensitivities, it is reasonable to assume that regional variations in temperature and humidity can significantly impact engine-out emission levels. These temperature and humidity variations are not fully accounted for in ambient air quality models used by states to assess the impact of various strategies for achieving the ambient air quality standards.

Historically, the impact of ambient temperature and humidity on emissions was of interest because it was impossible to make comparisons of the NO_x emissions from engines tested at different locations, or due to variations in the ambient conditions. In an effort to allow these day-to-day and location-to-location comparisons, various correction factors have been developed. The goal for all of these correction factors is to standardize the NO_x emissions back to selected standard reference conditions.

In light of the pressure on states and urban areas for implementing and achieving air quality standards, it seems appropriate to account for regional benefits or penalties imposed by prevailing ambient conditions. Of particular interest is the impact of ambient conditions on oxides of nitrogen (NO_x), a major contributor to ambient air ozone levels.

2.0 OBJECTIVE

The objectives of this project were to review existing data and correction procedures for adjusting diesel engine NO_x levels for ambient temperature and humidity, and to assess the applicability of these procedures for a number of different diesel engine categories that are used in the Houston Area.

3.0 APPROACH

The existing procedures for correcting NO_x emission levels for ambient temperature and humidity effects were reviewed. The Houston area population of diesel engines was reviewed and divided into subcategories for application of the various existing correction procedures. The correction procedures were compared to each other and to accepted engine performance and emission models for quantitative effects. Recommendations were then made on the application of the correction factors to the engine subcategories.

3.1 Existing NO_x Correction Procedures

A survey of the literature found four applicable procedures for adjusting NO_x emission levels for ambient temperature and humidity. Two procedures were for the heavy-duty diesel engine class (3-5), one for locomotives(6,7), and one for light-duty diesel engines(8).

The SAE correction factor for heavy-duty diesel engines was based on work performed by Krause, et al., in 1973(3). The relationship, presented as Equation 1, includes the effects of both temperature and humidity, and is referenced to standard conditions of 85°F (29.4°C) and 75 grains/lb (10.71 g/kg) humidity,

$$\begin{aligned} &KNOx = 1 + A(H-75) + B(T-85) \\ &Where: \\ &A = 0.044(F/A) - 0.0038 \\ &B = -0.116(F/A) + 0.0053 \end{aligned} \tag{1}$$

where F/A is the fuel-to-air ratio by mass. The SAE standards J177 and J1003 that reference this correction procedure were recently cancelled on October 1, 2002 with the comment that these procedures were no longer required. This correction factor was also, and continues to be, used as part of the EPA standards CFR title 40 part 89(4).

Note that the above methods require knowledge of the operational fuel-air ratio, a value that is not easily obtainable for a fleet of vehicles. Also, since these engines/vehicles operate over a wide range of conditions, selection of an average fuel-air ratio for general use would be difficult. Krause, et al., also presented a more generalized equation without the fuel-air ratio term. This equation is,

$$KNOx = 1 - 0.00216(H-75) + 0.00076(T-85) \tag{2}$$

Fritz (5) developed a correction for temperature and humidity based on measurements made in a number of modern (1998-1999) on-road truck engines. A characteristic of this class of engine is the use of air-to-air charge-air coolers. For this study, each manufacturer set up the air-to-air intercooler, which determines the relationship between ambient and charge air temperature. During testing, both the intake and manifold temperatures were controlled per the supplied relationships. This correction factor is shown in Equation 3.

$$\begin{aligned} &KNOx = 1 + \left[0.00446(T-25) - 0.018708(H-10.71)\right] \\ &where: \\ &T = ambient\ temperature,\ {}^{o}C \\ &H = ambient\ humidity,\ g/kg \end{aligned} \qquad (3)$$

Fritz and Dodge$^{(6)}$ developed correction factors for use with locomotive engines. The correction factors include both temperature and humidity parameters. This method was incorporated into the EPA regulations related to locomotive emission standards$^{(7)}$ and is presented in Equation 4. It is important to note the temperature term is actually the intake manifold temperature, not the ambient temperature, and thus the ambient effects are obscured by the generally unknown relationship between the intake manifold and ambient temperatures. The proposed rule incorporated an additional term in the final correction factor related to the uncertainty regarding the overall procedure.

$$K_H = \frac{C_1 + C_2 e^{(-0.0143)(10.714)}}{C_1 + C_2 e^{(-0.0143)(1000H)}} \qquad K_T = \frac{1}{1 - 0.017(T_{30} - T_A)}$$

Where:

$C_1 = -8.7 + 164.5e^{-0.0218(A/F)}$

$C_2 = 130.7 + 3941e^{-0.0248(A/F)}$

H = The specific humidity on a dry basis of the intake air (grams of water per kilogram of dry air).

(A/F) = Mass of moist air intake divided by mass of fuel intake.

T_{30} = The measured intake manifold air temperature in the locomotive when operated at 30°C.

T_A = The measured intake manifold air temperature in the locomotive as tested.

$$KNOx = \frac{1}{K_H K_T} \qquad (4) \qquad (4)$$

The effects of temperature and humidity on light-duty diesel engines were investigated by Hare and Bradow$^{(8)}$. This study included four naturally aspirated diesel engines with prechamber-style combustion chambers. The resulting correction for ambient conditions included only humidity effects, as the range of temperature variation was small; thus, no clear trend for ambient temperature effects was observed. The correction factor is shown in Equation 5.

$$\begin{aligned} &KNOx = 1 - 0.0152(H - 10.71) \\ &where: \\ &H = ambient\ humidity,\ g/kg \end{aligned} \tag{5}$$

The NO_x emissions are kinetically controlled during combustion and are fundamentally related to the composition of the fuel, and the time-temperature history during combustion through the adiabatic flame temperature. It is clear that the intake air temperature and humidity affect the adiabatic flame temperature through their impact on the chemical equilibrium conditions during combustion. The initial air temperature affects the compression temperature, which, in turn, affects the flame temperature. The humidity affects both the dilution of the mixture and the specific heat. In fact, these interactions are well understood and can be predicted reliably in a number of engine cycle simulation models.

Thus, in addition to the correction procedures found in the literature, ambient temperature and humidity effects can also be predicted using cycle simulation software. ALAMO_ENGINE(9) is a cycle simulation code that was developed at Southwest Research Institute that has been demonstrated to provide good predictions of the effects of fuel composition and intake mixture conditions and composition on changes in the NO_x emissions. These effects are accounted for in the model through the use of an adiabatic flame temperature calculation that is performed on a crankangle-resolved basis. The NO_x predictions made using ALAMO_ENGINE have been compared to engine test data, and the results have been good for a wide range of diesel engine designs (e.g., ref. 9).

3.2 Houston Area Diesel Engine Population

The diesel engines used in the Houston can be conveniently considered in terms of four different categories of application, and from two to three different technology levels in each category. They are:

3.2.1 Category 1 - On-Road

a. Pre-1994
b. 1994-2002
c. 2002-

3.2.2 Category 2 – Off-Road

a. Naturally Aspirated Construction/Farm (<50 HP)
b. Turbo Charged and Charge Cooled Construction/Farm (>50 HP)

3.2.3 Category 3 – Railroad

a. Two-Stroke Cycle Engines
b. Four-Stroke Cycle Engines

3.2.4 Category 4 – Marine

a. Generators
b. Main Propulsion

All of the correction factors presented above are based on the use of the ambient temperature and humidity, except for the railroad application, where the correction factor is based on the intake manifold conditions. The thermodynamic conditions of the intake air are affected by passage through the intake system.

The intake system can be conveniently considered in terms of two sections. The first section is from the ambient to the intake manifold, the second is from the manifold to the cylinder. The first section can be relatively simple, consisting of simply a filter and a pipe or plenum, typical of a naturally aspirated engine, such as categories 1a, 2a, and 4a listed above. Alternatively, the first section can also be very complex, including the use of an exhaust driven turbocharger compressor and heat exchanger. These configurations are exemplified by categories 1b, 2b, 3b, and 4b. The first section could also include the use of an engine-driven compressor, in addition to the turbocharger, exemplified by 3a.

In all of these cases, the first section affects the temperature of the intake air as it passes through the various devices. Additional changes are likely as the air passes through the second section, where it is affected by heat transfer from the hotter surfaces of the intake port and intake valve.

Every different engine design incorporates features that can, and probably do have different effects on the thermodynamic conditions of the intake air as it enters the engine. In this sense, every engine could theoretically have its own correction factors. The categories and sub-categories, listed above, were identified for this study because they represent, on average, the various combinations of engine technologies that may be affected differently by variation in the ambient temperature and humidity.

ALAMO_ENGINE was used to demonstrate the relative effects of intake manifold humidity, temperature, and EGR level. The results of these predictions are presented in Figures 1 and 2, where the NO_x predictions are plotted versus humidity and EGR level, at constant temperature, and versus humidity and intake temperature at zero EGR. Although there are very few EGR-equipped engines in the field today, it is important to predict the effect of ambient temperature and humidity on these engines to see if their response is dramatically different from non-EGR engines. The calculations were performed assuming that the engine was a 1998 12.7-liter DDC Series 60 engine, equipped with a turbocharger and charge-air cooler, but with the addition of EGR to bring the engine to 2002 standards. The conditions were assumed to be full load at 1800 rpm, with EGR levels that span a reasonable range for this load condition. Over a heavy-duty cycle, most of the NO_x is produced at the higher load conditions, so full load was chosen for these simulations. The intake manifold temperature and humidity ranges were selected to be representative of conditions at various times throughout the year in Houston.

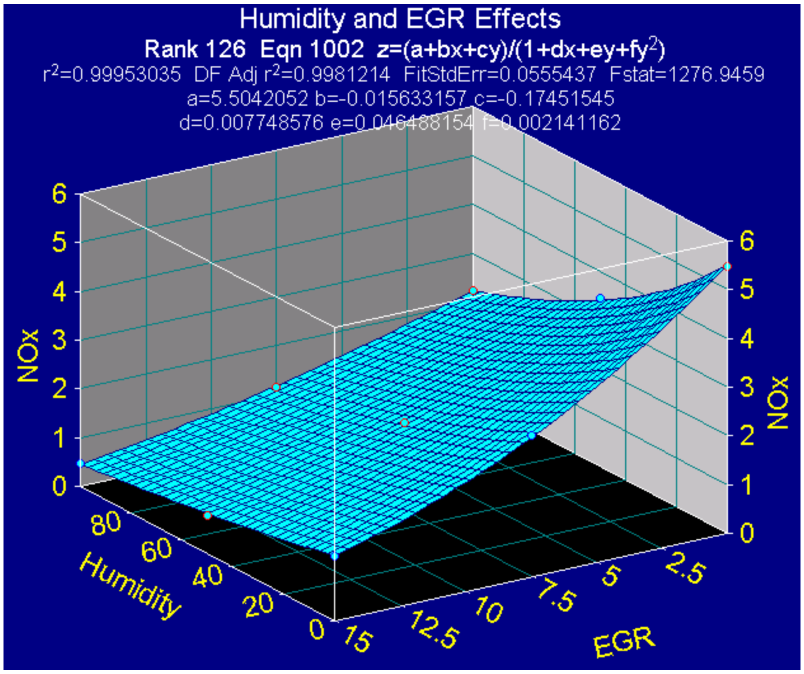

Figure 1 . Humidity and EGR Effects on NO_x - Model Results

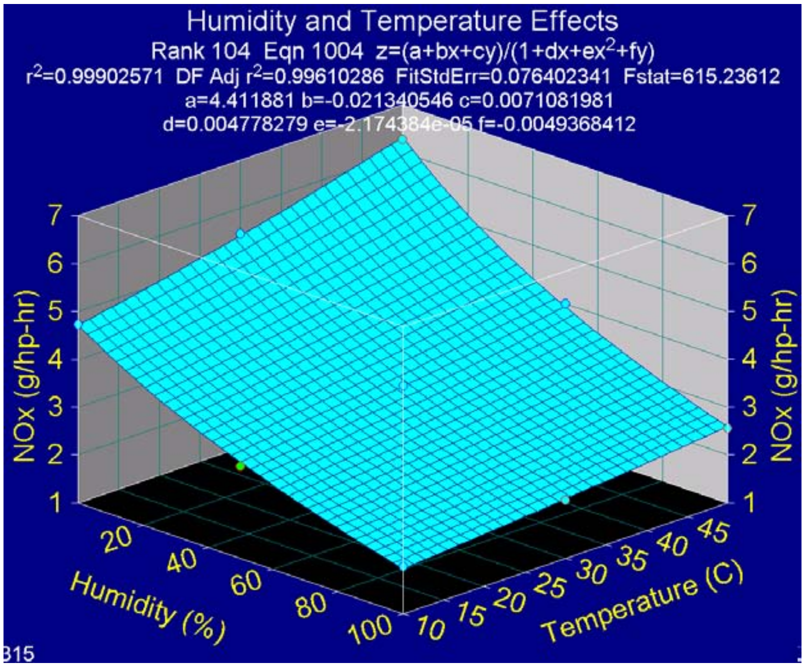

Figure 2. Humidity and Intake Manifold Temperature Effects on NO_x – Model Results

The results of the calculations indicate that the NO_x is affected by all of the parameters, with EGR and humidity having the largest effects. These predictions justify the need for the correction factors and also demonstrate the relative importance of the various parameters that are incorporated in the correction factor calculations.

3.3 Correction Factor Comparisons

As discussed briefly above, there are several problems with the existing correction procedures for ambient effects. First, it should be noted that only limited data for diesel engines were found in the literature. Two of the four studies, the light-duty(8) and EPA/SAE(3) heavy-duty procedures, were conducted in the 1970's and represent effects with engine technology of that time period. Second, two of the published procedures, the EPA/SAE(3) and the locomotive(6) procedures, require the use of fuel-air ratio as a predictor variable. While this is convenient for steady-state testing, application of this procedure for fleet emissions is problematic due the uncertainty of the operational fuel-air ratio. Third, the light-duty and the locomotive procedures are not functions of ambient temperature. The locomotive correction factor requires the use of the manifold air temperature that may be difficult to estimate due to the wide variation in locomotive cooling system configurations. Fundamentally, the manifold air temperature should be a better predictor of NO_x formation; however, the relationship between manifold air temperature and ambient temperature is not always straightforward, particularly with turbocharged, aftercooled engines. The light-duty procedure, which may be useful for naturally aspirated engines, does not incorporate a temperature variable due to the limited temperature range over which the data were collected. In spite of these limitations, the correction factors by the various methods are remarkably similar.

The four different correction factor calculations were incorporated into an EXCEL spreadsheet. The four equations were then used to calculate the correction factors as functions of ambient temperature and humidity. The results of these calculations are presented in Figure 3, where the correction factors are plotted versus the humidity, at constant temperature (25°C). For these comparisons, Equation 2 was used to represent the EPA correction procedure that is based on the work by Krause et al(3), since it does not require an air/fuel ratio. The results indicate that the four different methods are very similar. Also plotted in Figure 3 are the ALAMO_ENGINE predictions of the relative effects of humidity on the NO_x for a Series 60 12.7-liter engine at 25.5:1 AFR. As can be seen, the ALAMO_ENGINE predictions are similar to the published results but indicate a larger humidity effect than observed. The humidity effect is predicted to be slightly less at lighter loads. Although EGR dramatically lowers NO_x, the humidity effect on NO_x is predicted to be similar for EGR and non-EGR engines.

The effects of ambient temperature on the NO_x correction factors are presented in Figure 4. In this case, the calculated temperature effects are assuming that the ambient temperature change results in the same temperature change in the intake manifold, where the actual temperature change is less than the ambient temperature change. However, the magnitude of the change in the intake manifold temperature depends on whether the engine is turbocharged/intercooled, turbocharged but not intercooled, or naturally aspirated. There is a larger variation in the correction factors for ambient temperature than observed for humidity. It should be noted that, as discussed above, the light-duty and the locomotive correction factors are not a function of ambient temperature, and hence, show no effect. This could be misinterpreted to imply incorrectly, that for these classes of engine, ambient temperature has no effect. For the locomotive correction factor, a relationship between ambient and manifold temperature is required to account for ambient temperature variation. For the light-duty engine class, insufficient temperature range obscured the temperature effects when the correction factor method was developed. In the case of a naturally aspirated engine, the relative NO_x can be predicted using ALAMO_ENGINE by assuming that the manifold air temperature is equal to the ambient temperature. This estimated correction factor is illustrated in Figure 4. As shown, the modeled results are similar to the results obtained by Fritz (5) for the heavy-duty engine class. This approach would be considered a worst case approach, as the manifold temperature would not be expected to vary as widely as the ambient air temperature. Limited testing at SwRI has compared the change in ambient air temperature to the change in temperature at the intake port area (which should be the best predictor for changes in NO_x emissions) of a turbocharged intercooled engine, and a 50ºC change in inlet air temperature resulted in a 25ºC change in the temperature in the intake port.

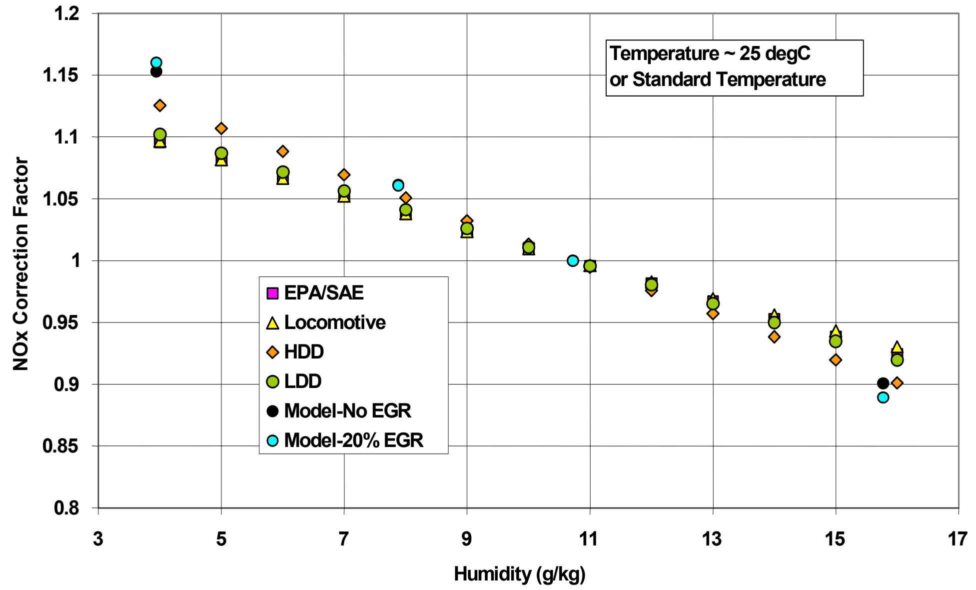

Figure 3. Humidity Effect on NO_x Correction Factors at Constant Temperature

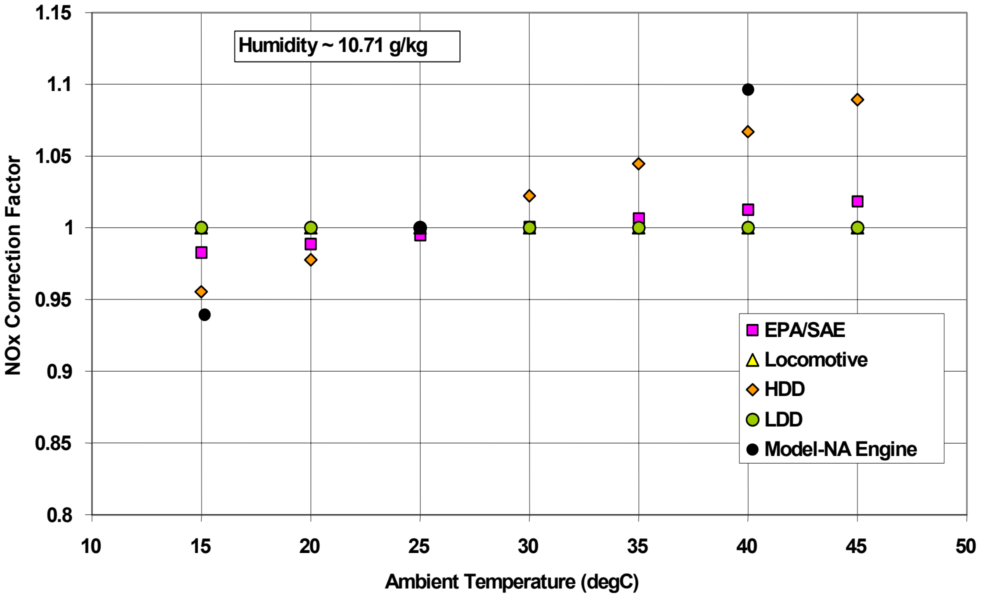

Figure 4 . Temperature Effect on NO_x Correction Factors at Constant Humidity

3.4 Recommended Practice

The variations in the correction factors are not large. The recommended approach is to apply the appropriate correction to each of the engine categories. This approach requires the existence of an inventory that includes the numbers and types of engines. It further requires that the engines in the inventory be categorized according to the scheme presented above. If this is done, then the correction factors should be applied as follows:

3.4.1 Category 1 - On-Road

a.	Pre-1994	Equation 2, essentially the EPA correction factor without the F/A ratio dependence. This eliminates the requirement for determining the F/A ratio of the fleet.
b.	1994-2002	Equation 3, heavy-duty correction procedures published by Fritz for late model diesel engines.
c.	2002-	Equation 3, heavy-duty correction procedures published by Fritz for late model diesel engines.

3.4.2 Category 2 – Off-Road

a. Naturally Aspirated Construction/Farm: The light-duty correction procedure, Equation 5, is not recommended for this class of engine due to the lack of temperature correction. Therefore Equation 2, essentially the EPA correction factor without the F/A ratio dependence, is recommended. This eliminates the requirement for determining the F/A ratio of the fleet.

b. Turbocharged and Charge-Cooled Construction/Farm: Equation 3, heavy-duty correction procedures published by Fritz for late model diesel engines.

3.4.3 Category 3 – Railroad

a. Two-Stroke Cycle Engines: Equation 4, the locomotive factors developed by Fritz. In order to use this equation, estimates of the F/A ratio and intake manifold temperature are required. If these values are not known, SwRI recommends an A/F ratio of 38, and no temperature correction (a value of 1.0 for this term of the equation).

b. Four-Stroke Cycle Engines Equation 4, the locomotive factors developed by Fritz. In order to use this equation, estimates of the F/A ratio and intake manifold temperature are required. If these values are not known, SwRI recommends an A/F ratio of 25.6, and no temperature correction (a value of 1.0 for this term of the equation).

3.4.4 Category 4 – Marine

a. Generators Equation 4, the locomotive factors developed by Fritz. In order to use this equation, estimates of the F/A ratio and intake manifold temperature are required. If these values are not known, SwRI recommends an A/F ratio of 38 for two-stroke engines, or 25.6 for four-stroke engines, and no temperature correction (a value of 1.0 for this term of the equation).

b. Main Propulsion Equation 4, the locomotive factors developed by Fritz. In order to use this equation, estimates of the F/A ratio and intake manifold temperature are required. If these values are not known, SwRI recommends an A/F ratio of 38, and no temperature correction (a value of 1.0 for this term of the equation).

4.0 SUMMARY

Existing correction procedures for ambient effects on NO_x emissions from diesel engine were reviewed. These procedures were developed for heavy-duty, light-duty, and locomotive diesel engines. In general, these procedures were similar in the effect of humidity, although the ambient temperature effects were not as clearly determined by the existing procedures. The defining temperature for NO_x emissions is the intake manifold air temperature, which is dependent on the ambient temperature but is also influenced by the engine configuration, turbocharged-aftercooled, naturally aspirated, or scavenged. Recommendations were made for application of existing correction procedures for the identified class of engines.

5.0 REFERENCES

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2. Manos, M.J., Bozek, J.W., Huls, T.A., “Effect of Laboratory Ambient Conditions on Exhaust Emissions”, SAE 720124, 1972.

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9. Dodge, L.G., Leone, D.M., Naegeli, D.W., Dickey, D.W., and Swenson, K.R., “A PC-Based Model for Predicting NOx Reductions in Diesel Engines,” SAE paper 962060, 1996.

APPENDIX B

Southwest Research Institute Report: “Humidity and Temperature Correction Factors For NO_x Emissions From Spark Ignited Engines”

HUMIDITY AND TEMPERATURE CORRECTION FACTORS FOR NO_X EMISSIONS FROM SPARK IGNITED ENGINES

FINAL REPORT

SwRI® Project No. 03.10038

Prepared for

ENVIRON International Corporation
101 Rowland Way, Suite 220
Novato, CA 94945-5010

October 2003

SOUTHWEST RESEARCH INSTITUTE®
SAN ANTONIO
HOUSTON
DETROIT
WASHINGTON, DC

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Engine, Emissions, and Vehicle Research Division

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EXECUTIVE SUMMARY

All of the current humidity correction factors for NO_x were found to be based on historical data taken in 1971 and 1972. Some of the engines today are more technically advanced than those engines, incorporating port or throttle-body fuel injection, air-fuel ratio feedback, exhaust aftertreatment, and knock detection. While many off-road vehicles do not have all of these features, this technology is becoming more prevalent in those engines as well. The analysis conducted for this project indicated that the historical correction factors do not adequately account for operating cycles with higher load factors, or advanced technologies such as A/F control and knock detection. No engine test data were found documenting humidity effects for these additional variables. Therefore, the recommendations given here were based on the correlations developed from engine tests conducted in the early 1970's, and the slopes for those correlations were adjusted based on engine modeling results that addressed the effect of higher load factors, A/F controlled to a constant value, and A/F fixed at a different value from the earlier tests.

The model results showed these effects to be significant and the results were used to modify the historical correction procedures. If a more rigorous approach is desired, SwRI would recommend engine testing to quantify the effects for different engine/vehicle classes.

The recommended equation to adjust standardized emissions for **carbureted heavy-duty on-road or off-road (above 19kW) engines** under non-standard inlet air conditions takes the following form:

$$C_{SwRI}(H,T) = 1 + 0.0022\cdot(T - 25) - 0.0280\cdot(H - 10.71) \qquad (13)$$

Where:
T = Temperature of the inlet air [^oC]
H =Absolute humidity of the inlet air [g of H_2O/kg of dry air]

For **heavy-duty on-road or off-road (above 19kW) spark-ignition engines that use a 3-way catalyst** (A/F control, typically with port fuel injectors), the recommended NO_x correction equation is as follows:

$$C_{SwRI}(H) = 1 - 0.0232\cdot(H - 10.71) \qquad (11)$$

with no correction for ambient temperature.

For **light-duty, spark-ignition engines**, the recommended practice is whatever procedure is used in Mobile 6, which can be approximated by Equation 4.

$$C = NOx_{corr\_MOBILE}(H_a) = \begin{cases} 1.2 \text{ if } H_a \le 20 \\ (-0.004\cdot H_a + 1.28) \text{ if } 20 < H_a < 120 \\ 0.8 \text{ if } H_a \ge 120 \end{cases} \qquad (4)$$

Where:
H_a = Absolute humidity of the inlet air [grains/lb]

For **small off-road, spark-ignition engines (< 19kW)**, the recommended practice is,

(14)

$$C = 1 - \frac{546}{AFR} \cdot (\omega - 0.01071)$$

Where:
AFR = Air-fuel ratio of the engine
ω= Absolute humidity of the inlet air [kg/kg]

1.0 BACKGROUND

Emission regulations continue to place additional restrictions on urban areas trying to achieve ambient air quality standards. Although ambient air quality standards are national, achieving the standards is a regional problem delegated to the states. However, the certification procedures for on-road and off-road spark-ignited engines are standardized without regard for regional variation in ambient conditions like temperature and humidity. As early as 1970(1), it was recognized that the concentration of oxides of nitrogen (NO_x) in engine exhaust is significantly affected by the thermodynamic conditions of the intake air. Specifically, the intake air temperature and humidity have the dominant effects(1)(2)(3). Because of these sensitivities, it is reasonable to assume regional variations in temperature and humidity can significantly impact engine-out emission levels. Emissions inventory models such as the Environmental Protection Agency's (EPA) MOBILE and NONROAD(4)(5)(6) have been developed to account for pollutants attributed to both on-road and off-road mobile sources. These models use local information to adjust the inventory based on average regional temperature and humidity for specific categories of engines.

Historically, the impact of ambient temperature and humidity on emissions was of interest because it was difficult to make comparisons of the NO_x emissions from engines tested at different locations and/or with variations in the ambient conditions. In an effort to allow these day-to-day and location-to-location comparisons, various correction factors have been developed. The goal for all of these correction factors is to standardize the NO_x emissions back to selected standard reference conditions, or to provide an adjustment to the emissions inventory models enabling a more accurate prediction of ambient air quality.

In light of the pressure on states and urban areas for implementing and achieving air quality standards, it seems appropriate to account for regional differences imposed by prevailing ambient conditions. Of particular interest is the impact of ambient conditions on oxides of nitrogen NO_x, a major contributor to ambient air ozone levels.

2.0 OBJECTIVE

The objectives of this project were to review existing data and correction procedures for adjusting spark-ignited Otto-cycle engine NO_x levels for ambient temperature and humidity, and to assess the applicability of these procedures for a number of different mobile sources.

3.0 APPROACH

The existing procedures for correcting NO_x emission levels during standardized tests for ambient temperature and humidity were reviewed, along with the original reference work that developed these procedures. The correction procedures were compared to each other and to accepted engine performance and emission models for quantitative effects. Recommendations were then made on the application of the correction factors to the engine subcategories. For the purpose of this text, the main category should be considered spark-ignited, Otto-cycle engines containing the subcategories: light-duty vehicles and engines, heavy-duty vehicles and engines, and off-road engines.

3.1 Existing NO_x Correction Procedures

A survey of standardized procedures found two methods for correcting ambient humidity and temperature during engine and vehicle tests. The first one is for heavy-duty engines, and the second is another used for light-duty on-road sources as well as off-road mobile sources such as recreational, small off-road, and marine SI engines. Current emissions models such as MOBILE6 and the model developed through the California Air Resource Board (CARB), EMFAC2002, were also explored to identify alternative methods currently in use to correct NOx for ambient temperature and humidity. Other correction algorithms have been developed for specialized cases, though not found in a standardized procedure.

3.1.1 Standardized Corrections

The EPA has promulgated the following correction factor (KH in English units and KH_{SI} in SI units) for NOx based on ambient humidity in multiple sections of CFR Title 40(7). The correction factor is based on work performed by Manos in 1973(2):

$$KH = \frac{1}{1 - .0047\cdot(H - 75)} \qquad KH_{SI} = \frac{1}{1 - .0329\cdot\left(H_{SI} - 10.71\right)} \qquad (1)$$

Where:
H = Absolute humidity of the inlet air [grains H_2O/pound dry air]
H_{SI} = Absolute humidity of the inlet air [grams H_2O/kg dry air]

The standard absolute humidity for the EPA is 75 grains/lb or 10.71 g/kg. These equations, in some form, are used in:

1. CFR Title 40 §86.144-94 for 1977 and later model year light-duty vehicles
2. CFR Title 40 §86.1342-90 for transient tests on Otto-cycle light-duty engines
3. CFR Title 40 §90.419 for small spark ignited off-road engines below 19kW
4. CFR Title 40 §91.419 for marine spark-ignited engines
5. CFR Title 40 §1051.501 for off-highway vehicles including ATV's and snowmobiles.

While the equation is consistent throughout Title 40, it should be noted that the use of the correction factor is not defined uniformly. In some instances KH is defined as a multiplicative correction factor to the NO concentration, while other sections define KH as the correction for the humidity effects on NO_2 formation. However, in practice, the applications of these correction factors have all been applied to the total NO_x emission numbers. Equation 1 has also been incorporated into SAE J1088, a test procedure for measuring gaseous emissions from small utility engines(8), and in the Texas Natural Resource Conservation Commission Technical Analysis Division specifications for vehicle exhaust gas analyzer systems(9). CARB has also uses this equation in their exhaust emissions standards and test procedures for 2001 model year and later spark-ignited marine engines(10) and small off-road engines(11). All of the previous procedures define KH be set to 1 for two-stroke-engines. This definition is not explained in the CFR, but Brereton and Bertrand explain that carbureted two-stroke handheld engines are particularly hard to characterize from a regulator perspective because of the erratic dependence exhaust emissions have on ambient temperature and humidity(12).

The original work performed by Manos tested eight vehicles based on the Federal Register Volume 30, Number 108. These vehicles were selected to represent the various engine configurations and carburetion systems found in the United States at that time. During the tests, humidity was varied from 20 to 180 grains of H_2O per pound of dry air (~2.85 to 25.2 g/kg); however, the regression analysis excluded the data above 120 grains per pound (~17.2 g/kg). The temperature range was determined in accordance with the Federal Register to be between 68 and 86 °F.

For gasoline-fueled heavy-duty engines, the EPA presents a correction factor for NO_x based on the humidity of the inlet air. This correction factor was established based on the work of Krause(3) in 1971. The vehicles were tested according to the Federal Heavy-Duty Test cycle and the resulting humidity correction can be calculated with the following equation:

$$KH_{HDV}(G) = 0.6272 + .00629 \cdot G - .0000176 \cdot G^2 \tag{2}$$

Where:
G = Absolute humidity of the inlet air [grains H_2O/pound dry air]

The promulgated correction is solely a function of the inlet air humidity. The original correction equation was a regression of the observed dependence of NO concentration in ppm on the inlet air humidity. The range of absolute humidities tested was from 20 to 110 grains/pound. Krause also established a correction equation for the mass emissions of NO_2 g/bhp-hr as seen in the following equation:

$$KH_{HDV\_NO2}(G) = 0.634 + .00654 \cdot G - .0000222 \cdot G^2 \tag{3}$$

Equations 2 and 3, in conjunction with NO_x emissions modeled in Southwest Research Institute's ALAMO_ENGINE cycle simulation computer model, have shown that correction factors established with concentration data and the corresponding mass-based emissions are similar. Therefore, a correction factor developed from concentration data imparts little error when applied to the mass-based emissions of an engine. Krause developed equations to correct carbon monoxide and unburned hydrocarbons emissions for ambient conditions, but the statistical correlation's were not as strong as those from which equations 2 and 3 were derived.

The correction factors shown in equations 1-3 are used to adjust measurements of NO_x to a reference humidity. The emission inventory models use correction factors in an inverse manner, to convert a standardized emissions rate to an actual rate. The equation and figures in the following sections are defined to adjust a standard emission rate to an actual rate based on ambient conditions.

3.1.2 EPA Emission Inventory Models

The emissions inventory models used by EPA and CARB correct NOx emissions based on the average ambient conditions during engine operation. Emission models have been developed for both on-road and off-road mobile sources. The NOx correction factor used for a light-duty gasoline vehicle in EPA's MOBILE6 is shown in the following equation(13) and Figure 1 (equation is estimated from figure provided in EPA documents):

$$NOx_{corr\_MOBILE}(H_a) := \left| \begin{array}{ll} 1.2 \ \text{ if } H_a \le 20 & \\ (-.004\cdot H_a + 1.28) \ \text{ if } 20 < H_a < 120 & \\ .8 \ \text{ if } H_a \ge 120 & \end{array} \right. \qquad (4)$$

Where:
H_a = Absolute humidity of the inlet air [grains/lb]

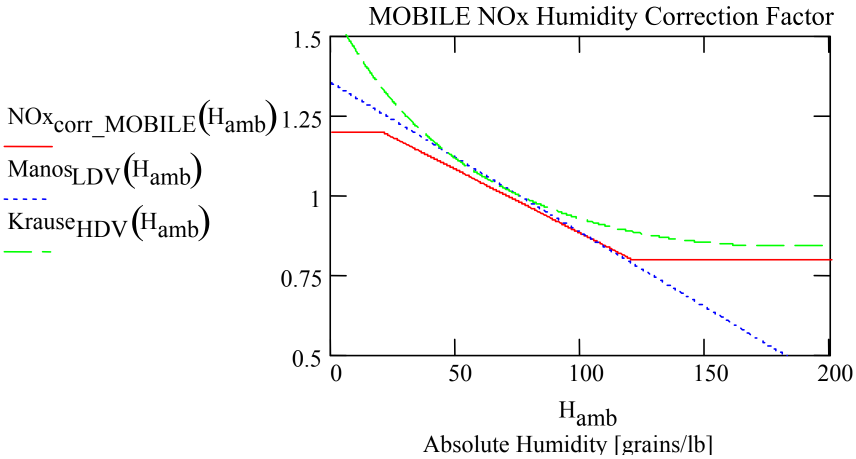

Figure 1. Humidity Correction Factors as a function of Intake Air Absolute Humidity for Three Cases: MOBILE6 (equation 6), Reciprocal of Manos Light-duty Vehicle (Equation 1), and Reciprocal of Krause Heavy-duty Vehicle (Equation 2).

Figure 1 shows three correction equations as a function of the inlet air humidity. While the empirical basis of the MOBILE6 function was not found, it appears to resemble the equation developed by Manos in the humidity ranges where the original regression analysis was performed. Continuing this speculation, it is probable that MOBILE6 model developers were not willing to extrapolate the Manos equation beyond the bounds of the regression analysis, and therefore, may not be accounting for the actual humidity effects on NO_x formation at high humidity.

Temperature correction factors in MOBILE6 are determined separately for each of the three segments of the FTP for light-duty gasoline fueled vehicles. For ambient temperatures below 75-°F the temperature correction factor (TCF) for NO_x emissions is as follows(4):

$$\mathrm{TCF}(b) = e^{[\mathrm{TC}(b)\cdot(T-75)]} \tag{5}$$

Where:
TC(b) = Coefficient for the particular test segment
T = Ambient temperature [°F]

TC(b) is dependent on the test segment, the ambient temperature, and the model year of the vehicle. At certain temperatures the TCF factor is combined with effects of fuel volatility as measured by the Reid vapor pressure. EPA's NONROAD2002, the off-road emissions model, calculates the correction factors with the same algorithm as MOBILE6, but with a matrix of TC(b) specific to off-road, four-stroke engines. NONROAD2002 does not apply a correction factor to two-stroke engine emissions due to a lack of data for these engine types.

3.1.3 CARB Emission Inventory Model

The CARB motor vehicle emission inventory model, EMFAC2002, corrects NO_x emissions for the ambient conditions where the vehicle/engine operates. CARB based their humidity correction methodology on that published by Manos. CARB expands on the original methodology by adding a factor that is determined by the technology class for a given vehicle. The technology classes are differentiated by the method of fueling, such as multi-point fuel injection or carburetion, and the exhaust aftertreatment. The factors were created through a linear regression analysis of data recorded between 1989 to 1995 including 885 light-duty trucks, 116 medium-duty vehicles and 3447 passenger vehicles ranging in model 1962 to 1995(6). The equation developed to estimate NO_x emissions for a vehicle operating at a humidity other than the standard 75 grains/pound takes the form:

$$E_{amb} = E_{Standard}\cdot\frac{\left(1 + m_{manos}\left(H_T - H_S\right)\right)\cdot\left(1 + m_{class}\left(H_{amb} - H_S\right)\right)}{1 + m_{class}\left(H_T - H_S\right)} \tag{6}$$

Where:
E_{amb} *= Corrected NOx mass emission*
$E_{Standard}$ *= NOx mass emissions at standard conditions*
m_{manos} *= -0.0047*
m_{class} *= ARB developed technology factors*
H_T *= Absolute humidity during the vehicle/ test [grains/lb]*
H_S *= Standard absolute humidity [grains/lb]*
H_{amb} *= Ambient absolute humidity during vehicle operation [grains/lb]*

The m_{class} factors were obtained through linear regressions. None of the published statistical R^2 values were larger than 0.033. Therefore, the adjusted correction has no statistical benefit over the original equation published by Manos.

EMFAC2002 corrects for the ambient temperature with technology specific correction factors for on-highway vehicles. The base equation takes the following form:

$$TCF = A\cdot(T-75) + B\cdot(T-75)^2 + C\cdot(T-75)^3 \tag{7}$$

Where:
A, B and C = Technology specific coefficients
T = Ambient temperature [°F]

Technology specific coefficients apply to the individual FTP segments and will adjust for engine differences such as fueling methods, exhaust aftertreatment, and air conditioning.

3.1.4 Specialized Corrections

The effects of ambient conditions on the performance and emissions of two-stroke and four-stroke hand-held engines were explored by Brereton and Bertrand. They established a correction that takes the form:

$$K_H = \frac{1}{1 - \frac{546}{AFR}\cdot(\omega - .01071)} \tag{8}$$

Where:
AFR = Air-fuel ratio of the engine
ω = Absolute humidity of the inlet air [kg/kg]

This equation accommodates the range of AFR (A/F) that a hand-held carbureted engine may experience in actual use. Equation 8, with an operating A/F of 16, will reduce to the form defined by the EPA for use with small off-road engines.

3.1.5 Comments on Current Correction Practices

Both the light-duty and heavy-duty correction equations, equations 1-3, were developed to correct for the minor variations in ambient humidity during a standardized test. The promulgated corrections are not suited for the wide range of humidity seen throughout the country. Use of any correction at conditions outside of the bound of the original regression should be considered an extrapolation. Equation 1, adopted by the EPA, did not include the effects of temperature because of the limited temperature range, and subsequent minimal effect on NO_x concentration. If the temperature adjustment is not removed from Manos' original equation to adjust an observed NO_x emissions to a standard humidity, it takes the following form:

$$Kh\left(T_{amb}, H_{amb}\right) := \frac{7.165}{\left[7.165 + 0.0290\cdot\left(T_{amb} - 78\right) - 0.0337\left(H_{amb} - 75\right)\right]} \tag{9}$$

Where:
T_{amb} *= Ambient temperature [°F]*
H_{amb} *= Absolute humidity of the inlet air [grains/lb]*

Figure 2 graphically represents Equation 9 for a range of possible ambient temperatures and humidities. The patch-marked and non-patch-marked sections of the figure delineate the regions of interpolation and extrapolation, respectively, when using equation 9. The area outside the bounds of the statistical analysis were explored with the cycle simulation code ALAMO_ENGINE to help characterized the validity of such extrapolations.

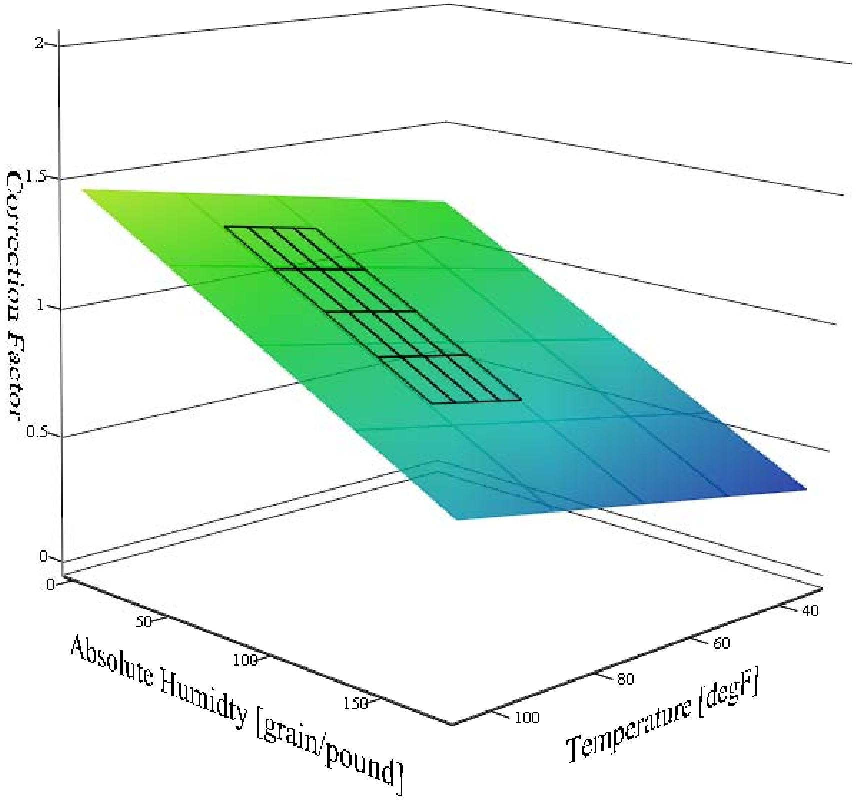

Figure 2. NO_x Correction Factor for Ambient Temperature and Humidity including the Bound of the Statistical Regression

The corrections presented in equations 1-3 were also developed on carbureted engines. The NO_x emissions from a carbureted engine will be affected by changes in humidity through three independent mechanisms. First, the water vapor in the intake will act as a diluent for the combustion charge, reducing the flame temperature, and therefore, the reaction rates for forming NO. Second, the diluent will slow the fuel burning rate, moving the average combustion later in the cycle where temperatures are lower due to the expansion cooling. (However, an engine with a knock sensor will not be affected in the same way.) Third, for a carbureted engine, an approximately fixed volume of air including humidity flows into the engine at a given throttle position. Water vapor displaces dry air, and therefore, increased humidity enrichens the (dry) A/F of the engine, which effects all engine emissions. Krause reported that a 100 [grain/lb] increase in humidity generally decreased the engine A/F by 0.4. The shift in A/F will have the most pronounced influence on NO_x formation if the engine is tuned to operate just lean of stoichiometric. Many light and heavy-duty vehicles operating today have tight A/F control to maintain the exhaust composition required for the aftertreatment process. Therefore, the NO_x emissions from these types of engines will not respond as strongly to ambient humidity changes as the carbureted engines did during the original testing of Manos and Krause. Figure 3 shows NO_x corrections based on Manos (Equation 1), Krause (Equation 2), and modeled results for both floating and fixed equivalence ratio.

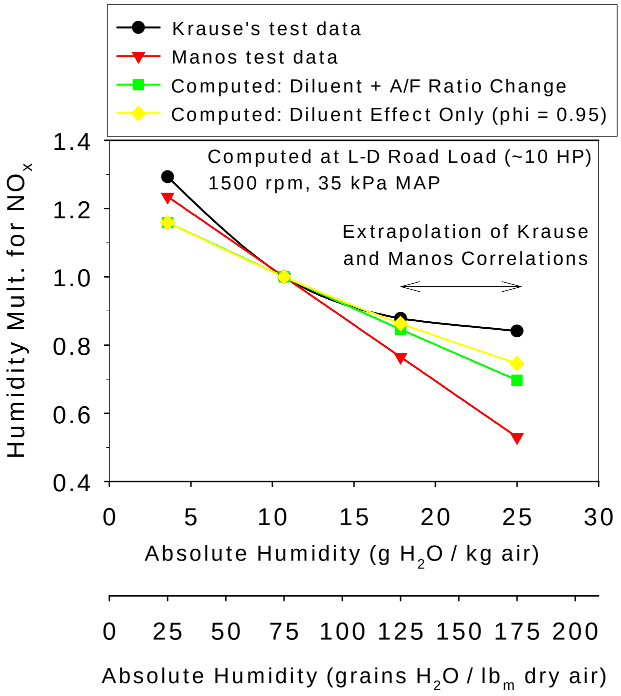

Figure 3. Humidity NO_X correction comparison

The modeled results were from the ALAMO_ENGINE code, which was developed at Southwest Research Institute. The details of how the ALAMO_ENGINE code computes power and NO_x emissions can be found in Appendix A. It should be noted that the humidity effects computed in ALAMO_ENGINE are based on solving chemical equilibria for the burning gases, computing the adiabatic flame temperature, and the kinetics for NO_x formation. Therefore, the computed results are not simply based on some humidity correction scheme, but rather on fundamental principles of the combustion process. The computed results are shown for two different cases. In the case labeled "diluent effect only," the A/F was fixed at 15.3 ($\Phi = 0.95$), and the humidity effect on the flame temperature through both the diluent effect and specific heat effect were accounted for. In the case labeled "diluent effect + A/F change," the A/F ratio was allowed to change from 15.5 at 25 grains/lb (3.6 g H_2O/kg dry air) to 15.3 at 75 grains/lb (10.7 g/kg), to 15.1 at 125 grains/lb (17.6 g/kg) to 14.9 at 175 grains/lb (25 g/kg). These changes in A/F were based on the test results reported by Krause. Therefore, both the change in A/F and the diluent effect were accounted for in this case. In all modern light-duty, on-road, gasoline engines, and most heavy-duty, on-road gasoline engines the A/F ratio remains fixed, independent of the humidity, since a sensor is used to maintain a fixed dry A/F.

As seen in the Figure 3, there is a significant discrepancy between the correction factors for humidity levels greater then 120 grains/lb. The second-order curvature of Krause's regression seems to under predict the slope of the correction factor at high humidity levels while the Manos equation may be over predicting the slope. Both the Manos et al, and Krause studies were conducted with engines that were subject to changes in A/F ratio with changes in humidity.

It should be noted that the ALAMO_ENGINE model results are for a single engine operating point (a light-duty, road-load of ~10 HP), while the data in the literature were for a combination of operating conditions. The sensitivity of the modeled NO_x to humidity was dependent on the engine operating conditions, with higher load conditions showing less sensitivity to humidity as shown in Figure 4. The model results also demonstrate that one would expect air-fuel ratio, or equivalence ratio, to effect the sensitivity of the NO_x emissions to humidity. If the engine is configured to operate rich of stoichiometric, the effect of humidity becomes less significant. Conversely, engines operating lean would be expected to demonstrate a larger sensitivity to humidity, as shown in Figure 5, where the modeling was performed at the Ford World-Wide Mapping Point (WWMP), a light load condition. The commonly used NO_x correction factors for ambient humidity do not account for these effects that could be important, depending on the application of the engine (light-duty or heavy-duty) and the engine fueling strategy (lean, stoichiometric, rich). The slope of the curves presented in Figures 4 and 5 represent the sensitivity of NO_x to ambient humidity. This slope is plotted versus the engine load (BMEP) and equivalence ratio in Figure 6.

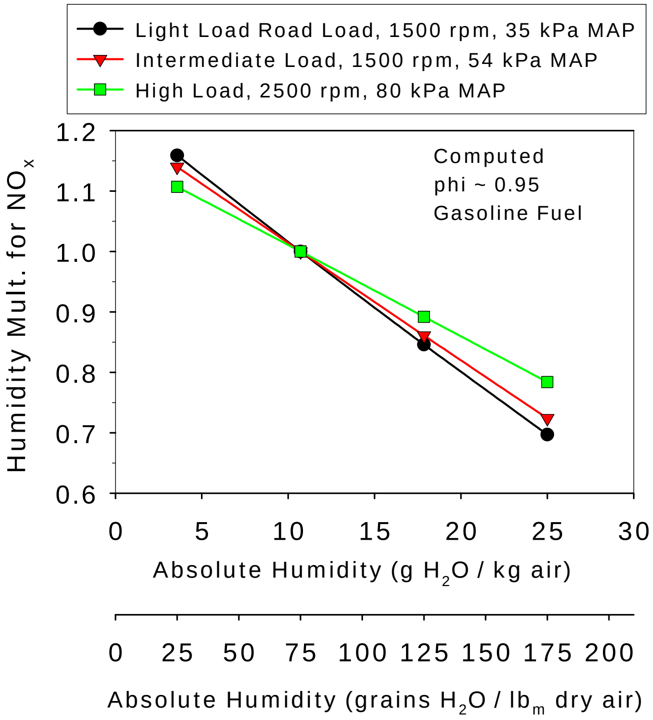

Figure 4. Effect of Load on Humidity Correction Factor

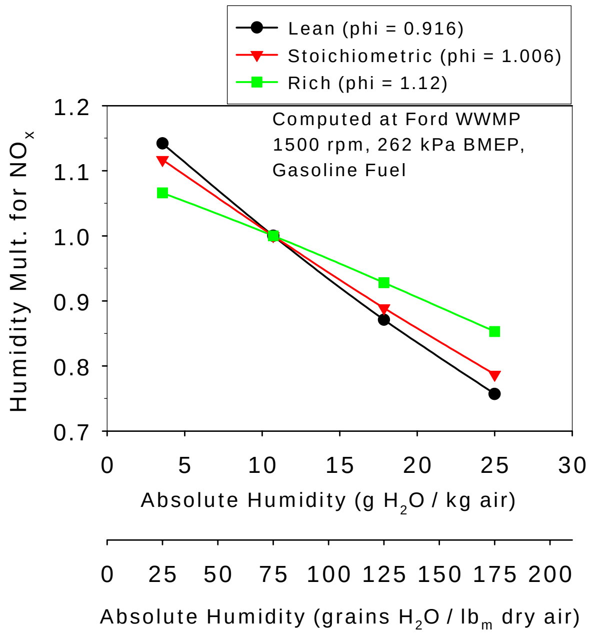

Figure 5. Effect of Equivalence Ratio on Humidity Correction Factor

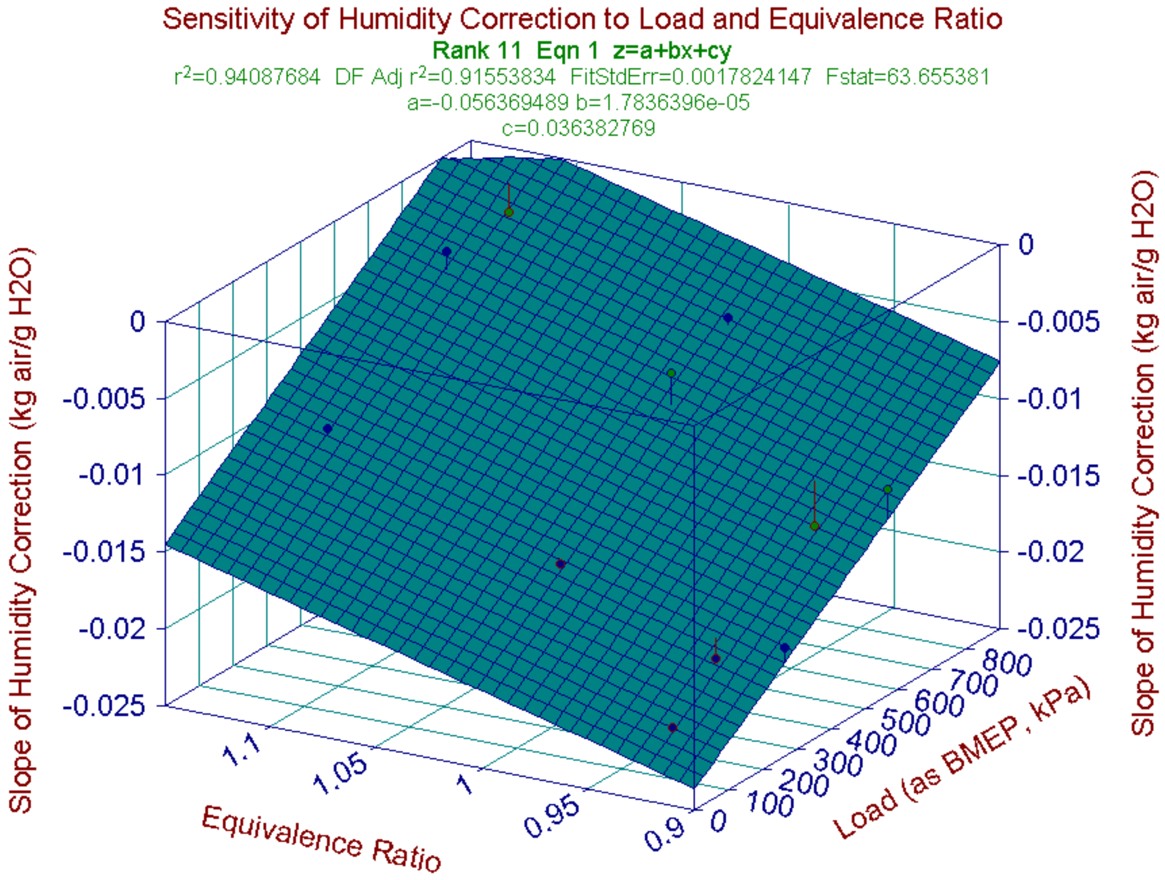

Figure 6. Humidity Correction as Function of Engine Load and Equivalence Ratio

All of the equations presented previously identify ambient conditions as the independent variable. However, it is the conditions present in the intake manifold that actually affect the NO_x formation. While the conditions in the intake manifold are coupled to the inlet conditions, the intake system will have an effect on the thermodynamic conditions presents in the intake manifold. The intake system can be conveniently considered in terms of two sections. The first section is from the ambient to the intake manifold, the second is from the manifold to the cylinder. The first section can be relatively simple, consisting of simply an air filter and a pipe or plenum, typical of a naturally aspirated engine, such as some on-highway and most small off-road engines. Alternatively, the first section can also be very complex, including the use of an exhaust driven turbocharger compressor and heat exchanger. These configurations can be found in large off-road stationary engines, and some on-highway applications. In all of these cases, the first section affects the temperature of the intake air as it passes through the various devices. Additional changes are likely as the air passes through the second section, where it is affected by heat transfer from the hotter surfaces of the intake port and intake valve.

Every different engine design incorporates features that can, and probably do have different effects on the thermodynamic conditions of the intake air as it enters the engine. In this sense, every engine could theoretically have its own correction factors. ALAMO_ENGINE was used to explore the effects of inlet humidity on NO_x formation for circumstances where there are no known standardized correction equations and to model emissions in the regime where other regression equations could only extrapolate. NO_x emissions were modeled with absolute humidity levels ranging from ~2.5 to 25 g/kg at different effective loads, and with multiple fuels. Figure 7 illustrates the humidity correction factor from ALAMO_ENGINE for propane and natural gas compared to gasoline at a light load under stoichiometric conditions. As indicated, under these conditions, propane and natural gas were slightly more sensitive to humidity than gasoline, although, recall that these are model results and not experimental data.

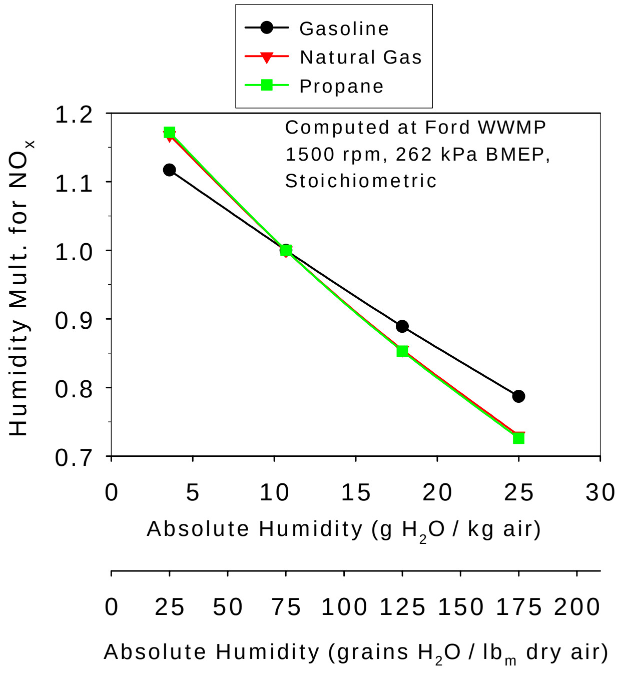

Figure 7. Fuel Effect on Humidity Correction

3.1.6. Effect of Air Conditioning Loads on Humidity and Temperature Correction Factors

Heavy-duty and off-road emissions tests are engine tests, not vehicle tests. Therefore, there is no allowance or concern for air-conditioner loads and their impact on emissions. Air conditioner compressors for passenger cars and trucks require about 1.2 kW (1.6 HP), a value which is likely negligible compared to the engine power required for heavy-duty engines used on a heavy-duty test cycle in vehicles large enough that they would use air conditioners. Air conditioners may have secondary impacts on the underhood temperatures, and this could impact NO_x emissions. These effects are too uncertain and too varied for any recommendations concerning humidity and temperature effects on NO_x emissions.

4.0 RECOMMENDED PRACTICES

4.1 Heavy-Duty On-Road and Off-Road Vehicles/Engines

The majority of gasoline heavy-duty on-highway engines and newer model off-highway heavy-duty engines operate with oxygen sensor feedback to control A/F just rich of stoichiometric to utilize the emission reduction benefits of three-way catalysts. Many also use knock sensors to tune the engine away from the detrimental effects of knock. An engine that is controlled to maintain a specific knock margin through EGR and ignition timing adjustments will also be reducing the humidity effect on burn rate. By reducing the effect of humidity on burn rate, the effect of humidity on NOx emissions will also be reduced. The current practices for adjusting NO_x emissions with intake air humidity do not incorporate any of these modern control practices into their theoretical methodology. Those practices that do correct based on technology classes seem to have extracted statistically irrelevant information from vehicle emission test databases. By modeling NO_x emission under a variety of conditions, SwRI was able to establish a theoretical revision of a standardized correction equation.

The approach taken here was to start with the test results and correlations developed by Manos et al.[2] and to make certain adjustments to the humidity correction factors suggested by them to account for the following effects:

1. Correct Manos et al.'s data from light-duty test cycles to heavy-duty test cycles.
2. For engines with closed-loop air-fuel ratio control, correct Manos et al.'s data taken on engines with variable air-fuel ratio to a fixed air-fuel ratio.
3. For engines with closed-loop air-fuel ratio control, correct Manos et al.'s data taken on engines with an average air-fuel ratio of 15.3 to a slightly rich of stoichiometric air-fuel ratio of 14.5.

For item 1, to establish a correction procedure for heavy-duty, on-road engines, and for off-road engines over 19 kW, which also operate at higher loads than light-duty applications, the correction procedure of Manos was selected as a baseline procedure. The correction developed by Manos was extrapolated to 175 grains/lb or 25 g/kg, and then the slope of the line was corrected based on theoretical modeling. Because the correction established by Manos was based on light-duty vehicles, the slope of the correction curve should be decreased by 15% due to the decrease in NO_x–humidity sensitivity at higher effective loads indicated by model results. Specifically, the percent change was calculated between the slope of the light-duty, road load in

Figure 4 and the average of the slopes for three loads, the light-duty road load, the Ford world wide mapping point (1500 rpm, 262 kPa BMEP), and the intermediate/high load point of 2500 rpm, 80 kPa intake manifold pressure (rough approximation of a HD cycle). Details are provided in Appendix B.

To account for item 2 above, engines with fixed air-fuel ratio control will not suffer the variable A/F ratio seen by Manos et al., and the resulting humidity effect on air-fuel ratio and on NOx. If the vehicle/engine class in question uses A/F control, the slope should be decreased another 10%. The derivation of this approximate correction factor is given in Appendix B.

To account for item 3 above, consider the following. The engines tested by Manos also operated at an A/F lean of stoichiometric, about 15.3. For engines operating near stoichiometric, 14.6, as typical for on-road, heavy-duty gasoline engines, the modeling study showed an approximately 9% reduction in the slope for the humidity correction factor. This may be seen qualitatively in Figure 5, and the quantitative analysis is given in Appendix B.

Therefore, the recommended equation to adjust standardized emissions for a carbureted heavy-duty on-road or off-road (above 19kW) engine under nonstandard inlet air conditions takes the following form:

$$C_{SwRI}(H) = 1 - 0.0280 \cdot (H - 10.71) \qquad (10)$$

Where:
$C_{SwRI} = NOx_{ambient}/NOx_{standard}$
H = Absolute humidity of the inlet air [g of H_2O/kg of dry air]

For heavy-duty on-road or off-road (above 19kW) engines that use 3-way catalysts (always with A/F control, and typically with port fuel injectors), the recommended NO_x correction equation is as follows:

$$C_{SwRI}(H) = 1 - 0.0232 \cdot (H - 10.71) \qquad (11)$$

Vehicles that utilize knock sensors in their engine control algorithms will further decrease their sensitivity to inlet humidity, though no data were found to quantify the magnitude.

Modeling results for heavy-duty engines running on either natural gas or propane show trends comparable to those seen for engines running on gasoline. Engine tests with natural gas fueled engines at SwRI have documented that humidity has an effect on NO_x emissions.(14) However, there is insufficient data on natural gas engines to specify a humidity correction factor for NO_x different from that for gasoline-fueled engines. Therefore, it is recommended that the same correction equations (Eq. 10 and 11) given above for gasoline engines should be used for propane and natural gas engines.

For heavy-duty engines that use carburetors and no aftertreament, Manos et al. measured a temperature effect on NO_x emissions. The ambient temperature affects the density of the air flowing through the carburetor, resulting in a shift in air-fuel ratio. The humidity effect on carbureted engines was quantified by Manos in Equation 9. Recall that Equation 9 would be used to correct to standard conditions and the inverse would be required to predict the effect of non-standard conditions. Using Equation 9 as the basis, the temperature correction term would then become:

$$C_{temp} = 0.0022 \cdot (T - 25) \qquad (12)$$

Where:

T = Temperature of the inlet air [^oC]

Applying this term to the humidity correction equation for carbureted engines (Equation 10) results in the following equation for NO_x correction that includes both temperature and humidity:

$$C_{SwRI}(H, T) = 1 + 0.0022\,(T - 25) - 0.0280 \cdot (H - 10.71) \qquad (13)$$

Where:

T = Temperature of the inlet air [^oC]

H =Absolute humidity of the inlet air [g of H_2O/kg of dry air]

For engines that have aftertreatment and accurate control of air-fuel ratio, the ambient temperature effect will be limited to effects on the charge air temperature, which is predominately determined by the manifold wall temperatures. Since this effect is largely unknown, it is recommended that no temperature correction be used for these engines.

To more accurately determine the correction factors for temperature and humidity, further testing is recommended to provide empirical data to clarify the apparent issues that this work could only address through theoretical modeling.

4.2 Light-Duty Vehicles

Unlike heavy-duty vehicles/engines the EPA corrects for the humidity effect on NO_x formation for light-duty, on-highway emissions in MOBILE6. For current modeling purposes, the recommended practice is Equation 4.

$$C = NOx_{corr\_MOBILE}(H_a) = \left|\begin{array}{l} 1.2 \ \text{ if } H_a \le 20 \\ (-0.004 \cdot H_a + 1.28) \ \text{ if } 20 < H_a < 120 \\ 0.8 \ \text{ if } H_a \ge 120 \end{array}\right. \qquad (4)$$

Where:

H_a = Absolute humidity of the inlet air [grains/lb]

This equation (in the region greater than 120 grain/lb and less than 20 grains/lb) should be modified based on empirical data as soon as valid testing is performed. The testing should also involve the technology classes present in the current inventories, to identify actual technology-based dependencies.

4.3 Small Off-Road Engines

For small off-road engines the recommended practice is Equation 8 for correcting observed NO_x emissions to a standard condition. To approximate a standard engine emission rate at non-standard conditions, the inverse of Equation 8 should be used. While the operating A/F may be difficult to estimate for the lawn and garden style engine inventory, test-cycle averages can be assumed. When the test cycle averages are not known, an estimate for the operating A/F of this class of gasoline engine is 12.0. For two-stroke engines, the NO_x correction factor should be set to 1.0 since no statistically significant dependence has been shown. The NO_x correction factor to estimate NO_x emissions at a non-standard condition from emissions data taken at standard conditions would then be,

$$C = 1 - \frac{546}{\mathrm{AFR}} \cdot (\omega - 0.01071) \tag{14}$$

Where:
AFR = Air-fuel ratio of the engine
ω = Absolute humidity of the inlet air [kg/kg]

5.0 SUMMARY

All of the current humidity correction factors for NO_X were found to be based on historical data taken in 1971 and 1972. Some of the engines today are more technically advanced, incorporating port or throttle-body fuel injection, air-fuel ratio feedback, exhaust aftertreatment, and knock detection. While many off-road vehicles do not have all of these features, this technology is becoming more prevalent. The analysis conducted indicated that the historical correction factors do not adequately account for operating cycles with higher load factors, or advanced technologies such as A/F control and knock detection. No engine test data were found documenting humidity effects for these additional variables.

The model results showed these effects to be significant and the results were used to modify the historical correction procedures. If a more rigorous approach is desired, SwRI would recommend engine testing to quantify the effects for different engine/vehicle classes.

The recommended equation to adjust standardized emissions for a **carbureted heavy-duty on-road or off-road (above 19kW) engine** under non-standard inlet air conditions takes the following form:

$$C_{SwRI}(H,T) = 1 + 0.0022\cdot(T-25) - 0.0280\cdot(H-10.71) \qquad (13)$$

Where:
T = Temperature of the inlet air [^oC]
H =Absolute humidity of the inlet air [g of H_2O/kg of dry air]

For **heavy-duty on-road or off-road (above 19kW) spark-ignition engines** that use a 3-way catalyst (A/F control, typically with port fuel injectors), the recommended NO_x correction equation is as follows:

$$C_{SwRI}(H) = 1 - 0.0232\cdot(H - 10.71) \qquad (11)$$

with no correction for ambient temperature.

For **light-duty, spark-ignition engines**, the recommended practice is whatever procedure is used in Mobile 6, which can be approximated by Equation 4.

$$C = NOx_{corr\_MOBILE}(H_a) = \begin{vmatrix} 1.2 \ \text{if } H_a \le 20 \\ (-0.004\cdot H_a + 1.28) \ \text{if } 20 < H_a < 120 \\ 0.8 \ \text{if } H_a \ge 120 \end{vmatrix} \qquad (4)$$

Where:
H_a = Absolute humidity of the inlet air [grains/lb]

For **small off-road, spark-ignition engines (< 19kW)**, the recommended practice is,

$$C = 1 - \frac{546}{AFR}\cdot(\omega - 0.01071) \qquad (14)$$

Where:
AFR = Air-fuel ratio of the engine
ω = Absolute humidity of the inlet air [kg/kg]

6.0 ACKNOWLEDGEMENTS

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APPENDIX A

ALAMO_ENGINE COMPUTER MODEL

ALAMO_ENGINE COMPUTER MODEL

An overall flow chart of the ALAMO_ENGINE computer model is shown in Figure A1. The model consists of three parts, a cycle simulation, a calculation of adiabatic flame temperatures and chemical species, and a submodel for computing NO_X emissions. Each of these submodels is briefly described below. A more complete description of the overall model as applied to diesel engine NO_X predictions was given previously by Dodge, et al. [A1].

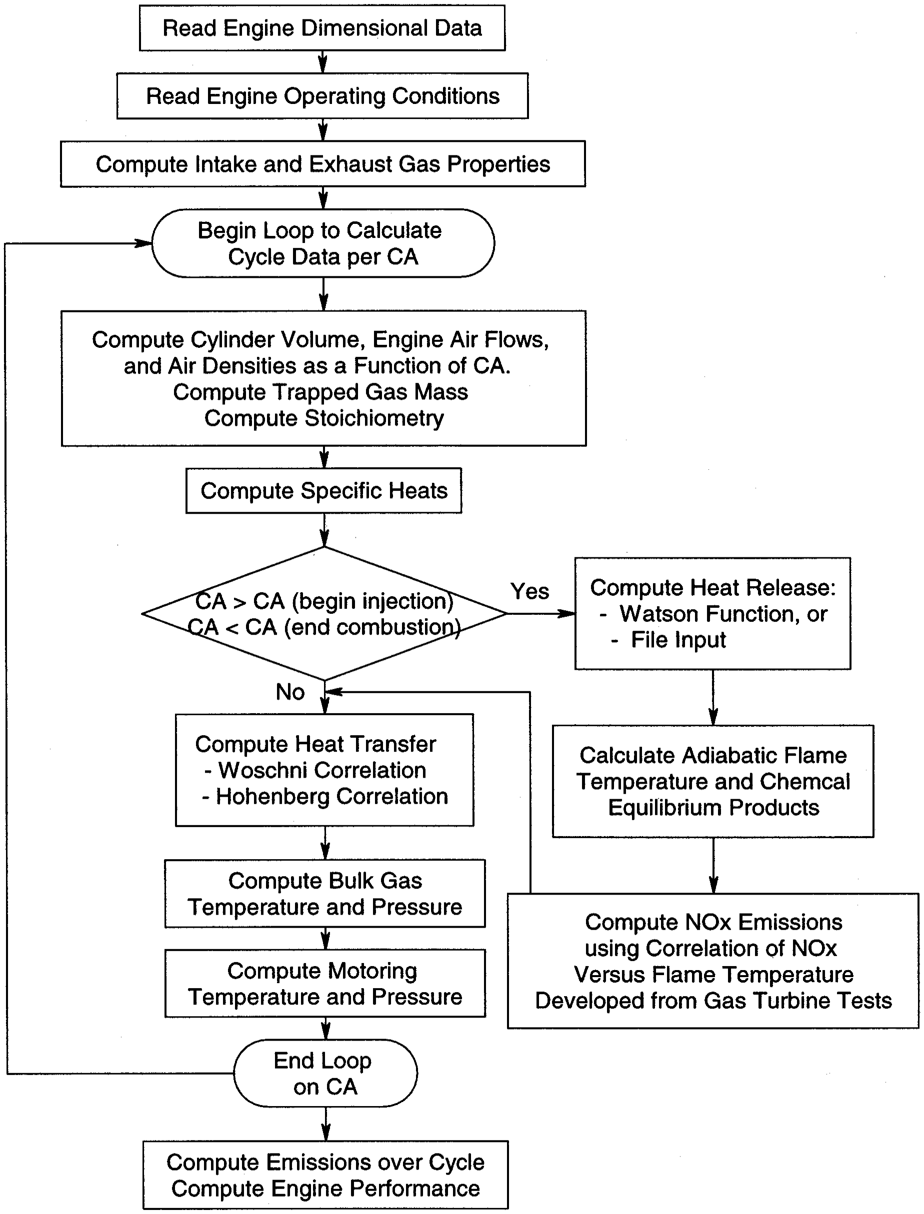

Figure A1. ALAMO_ENGINE Computer Model Flow Chart

CYCLE SIMULATION SUBMODEL

The cycle simulation portion of the model is fairly conventional with several added features for ease of use and to make it particularly suitable for studying combustion effects on NO_x. About 25 engines are stored in a database of engines that can be selected by the user. This database contains all the information required by the program to operate. Provisions are made in the program so that if some information about the engine is unknown, typical values for that size and type of engine are used. Heat release information can be estimated using a Wiebe function for spark-ignited engines or a modified Watson function [A1-A2] for compression ignition engines. Different Wiebe functions are selected for gasoline and natural gas engines to reflect the slower flame speeds of natural gas engines. If the apparent heat release rates have been measured, they may be used rather than the Wiebe or Watson correlations. Detailed gas compositions are computed for the unburned and burned gases based on equations given by Heywood [A3], so that the proper specific heats and other gas properties can be accounted for. The equations by Heywood were expanded to include water vapor from in-cylinder water injection and from emulsified fuels. This allows the program to evaluate the effect of EGR gases, residual gases, humidity, and water injection on NO_x emissions and power. Residual gas concentrations are calculated based on the work of Fox et al. [A4], as modified by Senecal et al. [A5] for turbocharged engines or by direct calculation of residual concentrations from the valve flow model. Residual gas temperatures are computed by iterating through the cycle simulation. The air flow through the engine is computed using a valve flow model. Heat transfer may be estimated from correlations developed by Woschni [A6] or Hohenberg [A7], or it may be turned off using the menu-based input. The Woschni [A6] heat transfer model was used for all calculations shown here, except as noted otherwise. The choice of heat transfer models can have a significant effect on NO_x and power predictions.

UNBURNED AND BURNED GAS TEMPERATURES SUBMODEL AND CHEMICAL EQUILIBRIUM SUBMODEL

The model assumes two in-cylinder gas zones, one for the unburned gas and one for the burned gas. (Shortcomings of this approach for predicting NO_x have been discussed by Raine et al. [A8].). In this approach, the burned gases are assumed to be fully mixed. The approach follows that of Heywood [A9]. The chemical equilibrium submodel was necessary to compute the equilibrium NO level as required by EQ. (6) below. The chemical equilibrium code was described previously by Dodge et al.[A1].

NITRIC OXIDES EMISSIONS MODEL

The NO_x emissions are calculated as NO based on the extended Zeldovich mechanism and a correlation for the Fenimore prompt NO mechanism. The results were summed together without consideration of further interaction. Even though the formation was assumed to be in the form of NO, conversions between NO_x concentrations in ppm and emissions rates expressed as g/HP-hr used the molecular weight for NO_2, in agreement with guidelines given by the U.S. Environmental Protection Agency. The well-known extended Zeldovich mechanism is given by [A10,A11]:

$$O + N_2 <=> NO + N \tag{1}$$

$$N + O_2 <=> NO + O \tag{2}$$

$$N + OH <=> NO + H \tag{3}$$

For the calculations reported here, the rate constants given by Heywood [A12] were used for the extended Zeldovich reactions. A correlation representing the Fenimore prompt NO mechanism is also used. [A13]

$$CH + N_2 <=> HCN + N \tag{4}$$

$$C_2 + N_2 <=> 2\ CN \tag{5}$$

The incorporation of the prompt NO mechanism into the model would have been difficult because of the requirement to add the hydrocarbon chemistry. However, Moore [A14] showed that the prompt NO correlates as a function of the equivalence ratio Φ, and the equilibrium nitric oxide concentration corresponding to the adiabatic flame temperature, $NO_{\text{equil. T adiab}}$

$$NO_{prompt} = f(\Phi)P^{1/2}NO_{\text{equil, T adiab}} \tag{6}$$

where P is the pressure in atmospheres, and Corr. et al. {A15] curve fit the data of Fenimore to get $f(\Phi)$ as,

$$f(\Phi) = 0.0053 \exp(1.004\ \Phi^{4.865}) \tag{7}$$

over a range of equivalence ratios from $0.8 < \Phi < 1.2$. Corr et al. [A15] extrapolated this function to $\Phi=0.6$ and got reasonable agreement with their data taken at that equivalence ratio. Both Corr et al. and Fenimore suggested that $f(\Phi)$ be multiplied by 0.75 in the case of methane combustion.

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APPENDIX B

DERIVATION OF CORRECTION EQUATIONS

DERIVATION OF CORRECTION EQUATIONS

This appendix shows the derivation of the amounts of correction required to apply Manos et al.'s experimental data and corrections to heavy-duty spark-ignition engines. Three potential corrections are required:

4. Correct Manos et al.'s data from light-duty test cycles to heavy-duty test cycles.
5. For engines with closed-loop air-fuel ratio control, correct Manos et al.'s data taken on engines with variable air-fuel ratio to a fixed air-fuel ratio.
6. For engines with closed-loop air-fuel ratio control, correct Manos et al.'s data taken on engines with an average air-fuel ratio of 15.3 to a slightly rich of stoichiometric air-fuel ratio of 14.5.

These corrections are approximate, and there are no test data that were found for comparison.

1. Correct Manos et al.'s data from light-duty test cycles to heavy-duty test cycles.
Consider the modeling results from three load conditions: light load, intermediate load, and high load. These data are presented in Figure 4 of the report. The corresponding slopes of the lines are shown in the table below. Application of the light duty correction equations to heavy-duty engines must account for the sensitivity of the humidity effect on load. To accomplish this, the slope of the humidity correction for light load compared to the average for the three cases. That is, the light-load data were assumed to correspond to the test conditions of Manos et al., while the average of the light, intermediate, and high load data were assumed to represent a heavy-duty test cycle. The term that resulted from the ratio was then used to adjust the humidity correction term from Equation 1 of the report.

Load Condition	Slope kg dry air/ g of H_2O
Light Load Road Load	-0.02159
Intermediate Load	-0.0194
High Load	-0.01506
Average	-0.01868
Light Load Road Load/Average	1.15

$$\frac{1}{KH_{SI}} = 1 - 0.0329(H - 10.71) \tag{1}$$

$$C_{SwRI}(H) = 1 - 0.0329 \cdot \frac{(-0.0187)}{(-0.0216)}(H - 10.71)$$

or

$$C_{SwRI}(H) = 1 - 0.0285(H - 10.71) \tag{10}$$

2. Correct Manos et al.'s data taken on engines with variable air-fuel ratio to a fixed air-fuel ratio (only applicable to engines with closed-loop air-fuel ratio control).

Equation 1 of the report was also derived from data for engines without air-fuel ratio control. Thus part of the correction accounted for variations in air-fuel ratio as humidity changed. For engines with air-fuel ratio control, the magnitude of this correction would be too large. To adjust for this difference, air-fuel ratio effects were modeled at an intermediate-load condition (the Ford world-wide mapping point of 1500 rpm, 262 kPa BMEP). These calculations were carried out simultaneous changes in humidity and corresponding changes in air-fuel ratio as observed by Krause[3] (0.4 A/F units per 100 grains of humidity change), and compared with changes in humidity with a fixed A/F ratio as observed by Krause of 15.3. For the engine with simultaneous changes in humidity and air-fuel ratio, the slope of the humidity correction was computed to be -0.02159, while for the engine with changes in humidity at constant air/fuel, the slope of the humidity correction was -0.01935. The ratio of these slopes is 0.896, or about a 10% reduction in humidity dependence if the air-fuel ratio is constant as compared to simultaneous changes in humidity and air-fuel ratio.

3. Correct Manos et al.'s data taken on engines with an average air-fuel ratio of 15.3 to a slightly rich of stoichiometric air-fuel ratio of 14.5 (only applicable to engines with closed-loop air-fuel ratio control).

These data are presented in Figure 5 of the report. The slopes of the line represented in Figure 5 for the lean (phi = 0.916) and stoichiometric (phi = 1.006) conditions are –0.0180 and –0.0154, respectively. This represents a 16.7% difference in slopes. The data used in the derivation of Equation 1 from Manos et al. were acquired for an equivalence ratio of approximately 0.95 (air/fuel = 15.3). In order to adjust the humidity coefficient in Equation 10, an interpolation of the humidity effect was used to determine the slope of a line at a 0.95 equivalence ratio. The slope was then used to adjust the humidity coefficient in equation 10 for a stoichiometric equivalence ratio.

$$slope_{0.95} = slope_{0.916} + (slope_{1.006} - slope_{0.916}) * \frac{(0.95-0.916)}{(1.006-0.916)}$$

$$slope_{0.95} = -0.0180 + (-0.0154 - (-0.0180)) * \frac{(0.95-0.916)}{(1.006-0.916)}$$

$$slope_{0.95} = -0.0170$$

$$\frac{slope_{1.006}}{slope_{0.95}} = 0.906$$

For engines with three-way catalysts, fixed air-fuel ratio control is used, and the engines are controlled to an equivalence ratio just rich of stoichiometric. Therefore, compared to Manos et al.'s humidity correction factor which was corrected in item 1 above for a heavy-duty cycle to a slope of -0.0285, the slope must be further reduced by the factors in items 2 and 3, or (–0.0285) (0.896) (0.906) = –0.0232. Therefore, for engines with fixed, stoichiometric air-fuel ratios, the humidity correction factor becomes,

$$C_{SwRI}(H) = 1 - 0.0232 \cdot (H - 10.71)$$