

Impacts of Natural Gas Composition on Air Quality – An Assessment Using TEMPLES Model

Provided to the California Air Resources Board

by

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Glossary

ARB:	Air Resources Board
BTU:	British Thermal Unit, unit of energy equivalent to 1055.06 Joules
CMAQ:	Community Multiscale Air Quality mode
CNG:	Compressed natural gas
CUC:	California Unified Cycle (driving cycle)
Emission Sensitivity Factor:	emissions change in a NG combustion device due to an increase in WI
FTP:	Federal Test Procedure (driving cycle)
Gs:	Specific gravity
HHV:	High heating value
LNG:	Liquefied natural gas
MN:	Methane number
NEI:	National Emissions Inventory
NG:	Natural gas
NMHC:	Non-methane hydrocarbons
NO _x :	Nitrogen oxides
PM _{2.5} :	Particulate matter with diameter smaller than 2.5 micrometers
SCC:	Standard Classification Code
scf:	Standard cubic feet
SMOKE:	Sparse Matrix Operational Kernel Emissions model
SoCalGas:	Southern California Gas Company
TEMPLES:	Tool for Emissions Processing of LNG Expansion Scenarios
tpd:	Short tons per day

USEPA:	United States Environmental Protection Agency
VERDI:	Visualization Environment for Rich Data Interpretation
WI:	Wobbe Index, in BTU/scf
WRF-ARW:	Advanced Research Weather Research and Forecasting Model
Δ WI:	Change in Wobbe Index, in BTU/scf

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Executive Summary

This report describes and demonstrates the use of a predictive model – the Tool for Emissions Processing of LNG Expansion Scenarios (TEMPLES) – to analyze how natural gas composition relates to air pollutants emission and statewide air quality.

TEMPLES comprises an emissions model (Sparse-Matrix Operational Kernel Emissions (SMOKE) model) and an air quality model (Community Multiscale Air Quality (CMAQ) model), to simulate air pollutant emissions and atmospheric transport and transformation of pollutants in the entire state of California. The modeling region extends to the entire state of California, with a model resolution in the horizontal plane of 4 km 4 km, and a vertical height of up to 10,000 meters above ground, with 30 layers of variable height based on pressure distribution. The emissions model uses the United States Environmental Protection Agency (USEPA) National Emissions Inventory data for 2005 as a baseline inventory, which includes all anthropogenic and biogenic sources of emissions. TEMPLES processes information on natural gas (NG) composition and emission factors from NG installations to determine perturbation in the emissions associated to NG combustion. Emission sources that are considered to be affected by natural gas composition and which are included in TEMPLES are residential, commercial and industrial natural gas combustion for space and water heating, cooking, electric power generation, industrial processes and transportation.

The simulated pollutant emissions and air quality impacts from changing natural gas composition depend on the assumed emission factor sensitivity for the technologies considered. The incremental change in natural gas quality is defined by the Wobbe Index, which is used in experimental studies as an indicator for NG quality. Values for emission changes per change in Wobbe Index are obtained from experimental studies of residential appliances for cooking, and water and space heating, commercial and industrial boilers, and light-duty and heavy-duty compressed natural gas (CNG) vehicles. The pollutant emissions included in the analyses depend on the source type, based on the data available from experimental studies. For residential sources, nitrogen oxide (NO_x) and CO emissions were reported, whereas for industrial and commercial installations only NO_x emissions were available. For mobile sources, NO_x, CO and non-methane hydrocarbons (NMHC) were reported and included in the analyses of CNG vehicles.

Three base cases and six scenarios, summarized in Table ES1, were developed to illustrate the capabilities of TEMPLES to determine the impacts of natural gas composition on emissions and air quality.

Table ES1 Simulation scenarios

Scenarios	Description
<i>Base Cases</i>	
Summer Baseline	Baseline emissions from the 2005 National Emissions Inventory for a week in July
Winter Baseline	Baseline emissions from the 2005 National Emissions Inventory for a week in December
CNG Base Case	Baseline emissions from the 2005 National Emissions Inventory for a week in July, assuming a CNG vehicle penetration of 5%
<i>Study Cases</i>	
Case A	Summer-time natural gas quality shift of $\Delta WI = +50$ BTU/scf for all stationary sources, with respect to Summer Baseline
Case B	Summer-time natural gas quality shift of $\Delta WI = +50$ BTU/scf for all stationary sources with maximum burner sensitivity for residential appliances, with respect to Summer Baseline
Case C	Impact of natural gas quality shift of $\Delta WI = +50$ BTU/scf for large electricity generation point sources only, with respect to Summer Baseline
Case D	Impact of LNG importation to San Diego County, with respect to Summer Baseline
Case E	Winter-time natural gas quality shift of $\Delta WI = +50$ BTU/scf, with respect to Winter Baseline
Case F	Summer-time natural gas quality shift of $\Delta WI = +50$ BTU/scf for CNG vehicles only, with respect to CNG Base Case

The three largest contributors to total NO_x emissions from NG combustion in the summer are industrial natural gas combustion from boilers and engines and commercial sector natural gas combustion. These sources are assumed to use low-NO_x burners which are

very sensitive to changes in Wobbe Index, and as a result, industrial and commercial sources are the main contributor NO_x emission increases in all cases where stationary sources are perturbed: Cases A-E.

Cases A and B produce the maximum increases in NO_x emissions for summer episodes, with increases of 63 and 64 tons per day, respectively. The difference between Case A and B is due to difference in emission sensitivity factors for residential appliances. Case E is winter-time case analogous to summertime Case B, and produces an increase in NO_x emissions of 71 tons per day. These emission increases correspond to approximately 2% of total statewide NO_x emissions in the year 2005. The emissions increase in the summer cases A and B causes 8-hour average ozone concentrations to increase by 1 ppb in sensitive areas like the San Joaquin and Sacramento Valleys. In addition, concentrations of PM_{2.5} increase by up to 0.3 µg/m³ in the Central Valley.

The effect of Wobbe Index in mobile sources is evaluated with the CNG Base Case and Case F. Both cases assume that 5% of all light-duty and heavy-duty vehicles are CNG vehicles. With this level of penetration, changes in Wobbe Index increase emissions of NO_x and NMHC by 23 and 45 tons per day, respectively. These emission increases correspond to 0.7% and 1.7% of all statewide emissions of NO_x and NMHC, respectively. This level of emission perturbations causes 8-hour average ozone and 24-hour average PM_{2.5} concentrations to increase by up to 0.6 ppb and 0.1 µg/m³, respectively.

These results demonstrate the applicability of TEMPLES to determine the effect of changing natural gas composition on pollutant emissions and air pollutant concentrations in California. Future work will implement Air Resources Board's 2012 emission inventory as the baseline to update the potential impacts of NG combustion sources. In addition, the impacts of natural gas composition on fugitive emissions from natural gas production, processing, transmission and distribution will be considered by incorporating new emissions sources into the TEMPLES model. These improvements will provide ARB with a unified model to evaluate changes in both statewide and local pollutant emissions and air quality due to changes in pipeline natural gas composition.

I Introduction

Owing to changes in natural gas (NG) sources the composition of NG used in California is changing, potentially increasing combustion emissions from NG equipment and engines. NG supplies may differ in composition (e.g., lower fraction of methane, higher fraction of ethane and other non-methane hydrocarbons) and properties (e.g., higher heating value and Wobbe index). Wobbe Index (WI) is particularly relevant as it is a measure of energy delivery to devices that control gas flow with a fixed orifice, and it is an indicator of interchangeability of fuel gases. It is defined by:

$$WI = \frac{HHV}{\sqrt{G_s}} \quad (1)$$

where HHV and G_s are the higher heating value and the specific gravity of the gas, respectively. Typical WI values in the NG system are around 1335 BTU/scf (British thermal unit per standard cubic foot of natural gas) and the maximum set by the California Public Utility Commission (CPUC) is 1385 BTU/scf.

Previous experimental results showed sensitivity in the emissions of nitrogen oxides (NO_x) and other pollutants from NG combustion applications due to changes in WI (SoCalGas, 2006a-c; Singer *et al.* 2009; Crawford and Lyons, 2009; Crawford and Lyons 2010).

Changes in NO_x emissions affect ozone and particulate matter formation and could impact efforts of air pollution control strategies to attain ozone standards in California.

Approximately 5% of NO_x emissions in California are produced by NG combustion in the residential, commercial, industrial, and utilities sectors (California Air Resources Board, 2009b), but the contribution from NG combustion to total emissions could change due to changes in NG composition.

This project developed a predictive model to analyze how natural gas composition relates to pollutant emissions and air quality, and provides the California Air Resources Board (ARB) with a tool to help assess the cost effectiveness of emissions reduction options. The model was originally devised to assess emissions impacts from changes in natural gas (NG) quality due to importing liquefied natural gas (LNG) into California. Because of the initial focus on LNG, the model was named Tool for Emissions Processing of LNG Expansion Scenarios (TEMPLES). Recent changes in the US NG market have virtually eliminated LNG imports into California. However, other sources of NG, such as domestic shale gas and biogas, may affect the quality and composition of natural gas, and can be studied by the TEMPLES model.

TEMPLES is developed with the objective of analyzing potential emission perturbations in the emissions from NG combustions. This report documents the model components, structure, and input requirements for TEMPLES, and includes demonstrations of TEMPLES in a series of scenarios that illustrate the model capabilities.

II Model Description

The TEMPLES model comprises three main modules: (1) an emissions model, (2) an air quality model and (3) a visualization package. The emissions model is based on the Sparse Matrix Operational Kernel Emissions (SMOKE) model. SMOKE is integrated in a custom-made program that receives input parameters related to natural gas composition and calculates the resulting emissions due to changes in gas composition. The air quality model module uses the community-developed Community Multiscale Air Quality (CMAQ) model and the post-processing tool to visualize results is the Visualization Environment for Rich Data Interpretation (VERDI) package, which are both publicly available. Figure 1 illustrates the main components of the modeling framework. TEMPLES refers to the three modules – Emissions Modeling, Air Quality Modeling, and Visualization Tools – and the inputs required to run the modules: Baseline Emissions Inventory and NG Distribution Scenarios parameters.

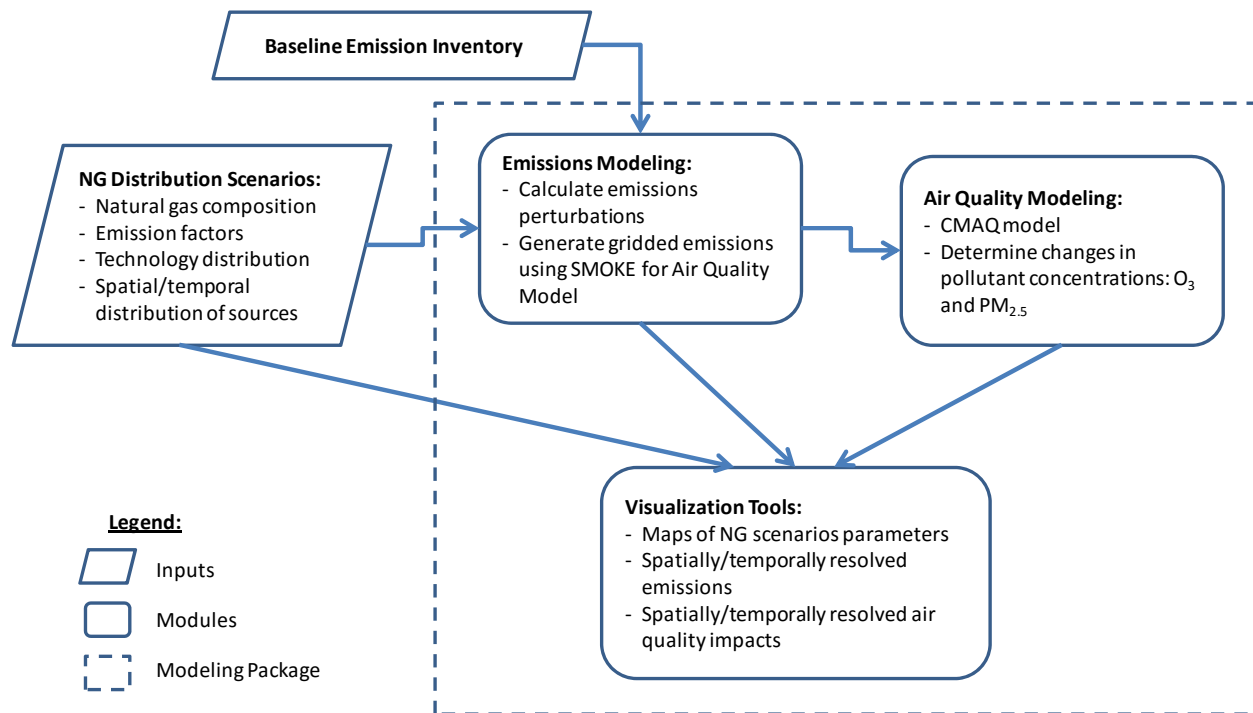


Figure 1 Components for the TEMPLES modeling framework.

Figure 2 illustrates the workflow and transfer of information within the TEMPLES modeling framework. In summary, the parameters input by the user (**Natural Gas δ** ,

Impact Scenario) are processed using the **Custom Pre-Processor** to apply emission perturbations to the **Base Inventory**. The resulting emissions (**Emissions***) are then input to the **Air Quality Model (CMAQ)**, which uses other inputs provided with TEMPLES (grey boxes). The results from the Air Quality Model (**Case Outcomes**), which are hourly and spatially-resolved concentration fields of pollutants, can be processed with the **Post-Processor (VERDI)** to obtain air pollution maps.

User interaction with TEMPLES is limited to two main tasks (shown in yellow boxes):

- 1) Input parameters that define a Test Case: changes in natural gas quality (defined by Δ WI), emission factors and emission sensitivity factors, and technology distribution factors.
- 2) Run the Post-Processor tool VERDI using the outputs generated by the air quality model (Case Outcomes)

In the following sections, the general concepts of the two modeling parts – emissions modeling and air quality modeling – and the description of inputs parameters are explained in more detail. The primary purpose of TEMPLES is to evaluate the air quality and emissions impacts of changing natural gas quality. In a typical simulation, many input data (shown in grey boxes in Figure 2) will not be modified by the user so that natural gas quality can be isolated as the only changing variable. Therefore, users are provided with pre-loaded data relevant to California geography, atmospheric chemistry, and meteorology. Thus, these components are not discussed in detail; the user can visit the Community Modeling and Analysis Center website (CMAS; <http://www.cmascenter.org>) for more details on these components. Appendix A includes a user's manual for TEMPLES.

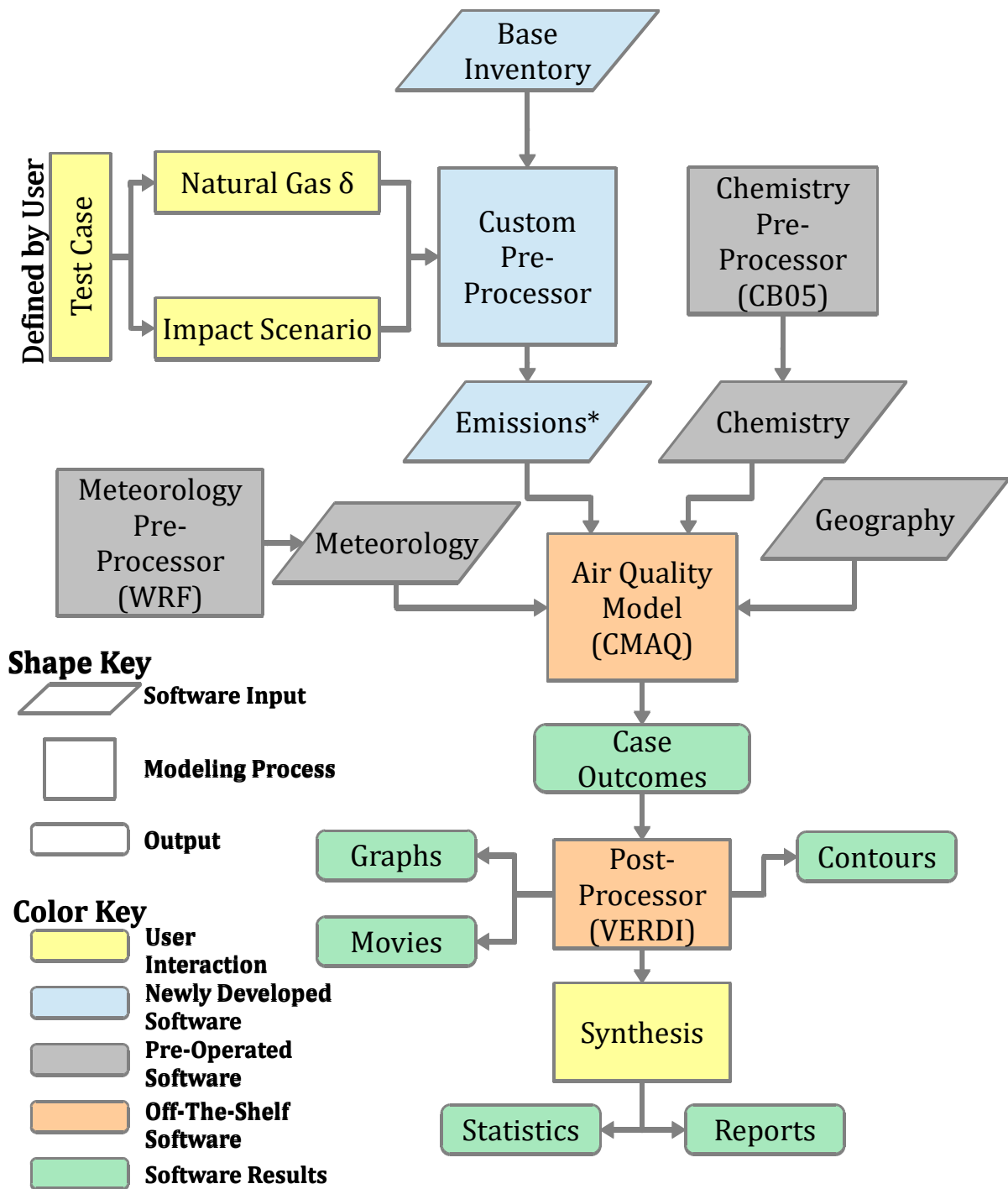


Figure 2 Detailed TEMPLES air quality model flowchart..

II.A Emissions Modeling

The emissions modeling part – executed by the Custom Pre-Processor – consists in processing of a set of input parameters that define a Test Case, to produce a perturbation in a Base Inventory of emissions due to natural gas composition changes, and generating the temporally-resolved gridded emissions that are required by the Air Quality Model (CMAQ). The Base Inventory is supplied with the natural gas tool and does not require direct user manipulation; it is based on the National Emissions Inventory for 2005 (U.S. EPA, 2011).

To define the test case, the user must be familiar with the type of emission sources considered in the inventory and the input data needed to define the case completely. The Custom Pre-Processor is built upon the SMOKE model (www.smoke-model.org), which accounts for all anthropogenic and biogenic emission sources. The types of sources that are relevant to the analysis of emissions from natural gas combustion are the following:

Point Sources: Point sources are large pollutant sources that are emitted from a single point, such as a stack at a factory. Emissions from these sources are reported to local air districts. Examples of point sources are electricity plants, refineries, and factories. In addition to latitude and longitude, the location of a point source includes elevation, and stack height and vertical plume rise are considered when determining the elevation of a point source.

Area Sources: Area sources are small pollutant sources that are spread over a geographical area and do not emit from a single location. These sources are individually much smaller than the industrial sources categorized as point sources, but the large number of area sources. Examples include residential cooking and small commercial and industrial processes. Data for area source emissions are aggregated for a region such as a city, county, or district. The resolution of the aggregation area often depends on the activity density within the region and the availability of monitoring station data within the area. Emissions reported as area sources are the aggregate of all emissions sources within the specified area. Vehicles have a separate source designation and are not included in area sources.

On-Road Mobile Sources: This source type includes all vehicles traveling on highways, streets and roads. The base emissions inventory includes the estimated vehicle fleet size and the total vehicle miles traveled within the state of California.

The Custom Pre-Processor is designed to apply emission sensitivity factors obtained from emission testing to the relevant emission source types described above. Emission testing is performed on specific NG applications (e.g. oven burner, premix power surface burner boiler, CNG Honda Civic), whereas emission sources included in the inventory are more generic (e.g. residential NG combustion, commercial space heating, light-duty vehicles). Consequently, the Custom Pre-Processor requires additional inputs that define technology distribution factors to link emission testing emission sensitivity factors with the emission sources present in the inventory. Section II.A.1 describes the emission sensitivity factors used in this study, and section II.A.2 presents the methodology to apply emission sensitivity factors to emissions in the inventory.

II.A.1 Emission Factors from Combustion of Natural Gas and Sensitivity to Natural Gas Composition Changes

The impacts of natural gas composition changes determined by TEMPLES depend on the assumed emission factor sensitivity for the technologies considered. These values are obtained from experimental studies conducted to determine emission changes due to changes in gas composition or WI.

The changes in emissions per change in WI are categorized for three different source types: residential sources, commercial and industrial sources, and mobile sources.

1) Residential Sources

The emission factors and perturbations due to changes in WI for residential sources are based on extensive emission testing conducted by the Lawrence Berkeley National Laboratory, LBNL (Singer *et al.* 2009). Various residential appliances were tested to determine changes in criteria pollutant emissions due to changes in WI. A thorough statistical analysis to determine emission factors and uncertainty bounds for those residential appliances is presented in Appendix B. Based on the statistical analysis of all measurements conducted by LBNL, two sets of emission sensitivity factors were calculated based on experimental probability distribution and interval of confidence. Table 1 presents the baseline emission factors for CO and NO_x and the two sets of emission sensitivity factors, the Best Engineering Estimate values and the Maximum Likely Increase values. For details on the statistical analysis, refer to Appendix B.

Table 1 Baseline emissions factors ($ef_{ij,l}$) and emission sensitivity factors ($\Delta ef_{ij,l}$) for residential burners.

	Emission Sensitivity Factor					
	Baseline Emission Factor (ng/J)		Best Engineering Estimate (ng/J per 50 BTU/scf increase in WI)		Maximum Likely Increase (ng/J per 50 BTU/scf increase in WI)	
	CO	NO _x	CO	NO _x	CO	NO _x
Cooktops	118.0	34.7	22.16	0.78	66.40	1.64
Broilers	97.0	29.3	12.34	0.66	34.10	3.08
Ovens	117.4	34.5	25.10	-0.36	52.04	1.00
Furnaces	12.9	29.2	-1.50	1.20	3.26	3.06
Storage Water heaters	0.1	25.6	0.38	0.24	1.98	1.26
Tankless Water Heaters	129.3	20.4	7.88	3.48	76.28	10.50

2) Commercial and Industrial Sources

In contrast to residential appliances, data on the effect of gas composition in commercial and industrial sources are limited. Emission tests were performed on low-NO_x (SoCalGas, 2006a, 2006b) and ultra-low-NO_x burners (SoCalGas, 2006c). In the experiments with low-NO_x burners, two types of steam boilers were used: (1) a 645,000 BTU/hr boiler, with a premix power surface burner type, which is the most common burner type in the SoCalGas service territory, and (2) a 397,000 BTU/hr boiler with premixed gun-type power burner, which industry experts claimed might be sensitive to rich gases. The emission testing included tuning the boilers to the baseline gas so that they met emission standards, and then measuring emissions when combusting two gases with WI values different from the baseline gas. For example, for the power surface burner, equipment was tuned to meet the emission specifications for NG with WI values of 1278 and 1342 BTU/scf, and then the burner was operated on NG with different WI values (SoCalGas, 2006a). Figure 3a presents the NO_x emission results of these experiments. Similar tests were conducted for the

premixed gun-type power burner, with the boiler tuned to NG with WI values of 1278 and 1434 BTU/scf, and those results are presented Figure 3b (SoCalGas, 2006b). Interpolation of this data for low-NO_x burners shows that NO_x emissions increase by up to 40% for a WI increase from 1335 to 1385 BTU/scf.

A boiler with a 645,000 BTU/hr surface premix power burner was used in experimental emission testing of ultra-low-NO_x burners (SoCalGas, 2004). Emission controls for this ultra-low NO_x burner are more sophisticated and complex than the controls in the low-NO_x burners in order to meet more stringent emission specifications. This more advanced technology could make the equipment more sensitive to changes in natural gas composition. The experimental data for the ultra-low NO_x burner is presented in Figure 4; the measurements showed an increase in NO_x emissions of 15% for a WI increase from 1335 to 1385 BTU/scf. Table 2 summarizes the emission sensitivity factors ($\Delta ef_{i,j,l}$) for commercial and industrial burners that are used in this study.

Based on an internal equipment survey conducted by the South Coast Air Quality Management District (Baez, 2010), commercial and industrial area sources are typically smaller units with low-NO_x burner technology, and commercial and industrial point sources are usually large equipment with ultra-low NO_x technologies.

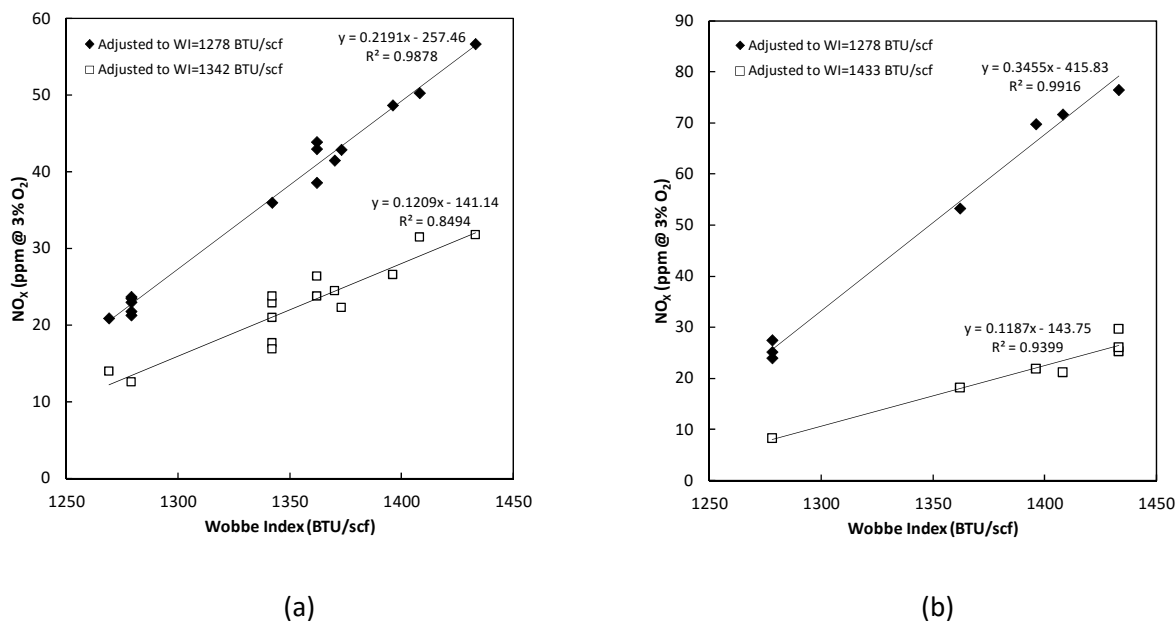


Figure 3 Measured NO_x emissions versus WI for commercial and industrial burners: (a) steam boiler with premixed gun-type power burner (SoCalGas, 2006a), (b) low-NO_x steam boiler (SoCalGas, 2006b).

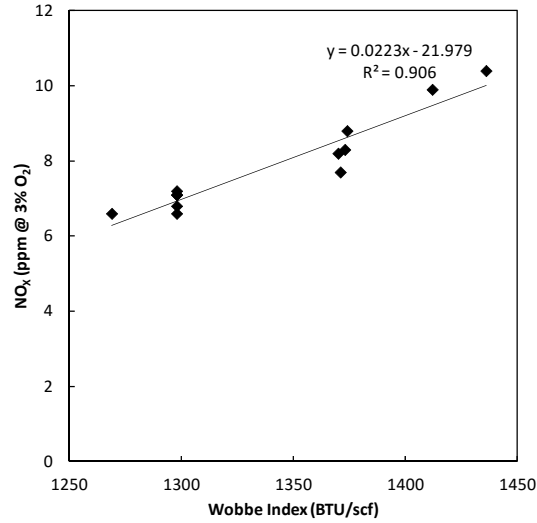


Figure 4 Measured NO_x emissions versus WI for an industrial ultra-low NO_x steam boiler (SoCalGas, 2004).

Table 2 Emission sensitivity factors ($\Delta ef_{i,j,l}$) for commercial and industrial burners.

Burner Type	NO _x
	Emission Sensitivity
	Factor
	(% per 50 BTU/scf increase in WI)
Low-NO _x burner	40%
Ultralow-NO _x burner	15%

Additional information on emissions from industrial and commercial applications is found in reports conducted by the Gas Technology Institute (GTI, 2006; Tickel *et al.* 2009; Tickel and Wagner, 2009). This information will be analyzed following the same methodology used for residential appliances (Martinez *et al.* 2014) and incorporated into the model to provide a more statistically grounded range in the emission sensitivity factors for industrial and commercial equipment.

All the data presented above for industrial sources is related to boilers and burners. There is very limited information on the sensitivity of gas turbines and other stationary internal

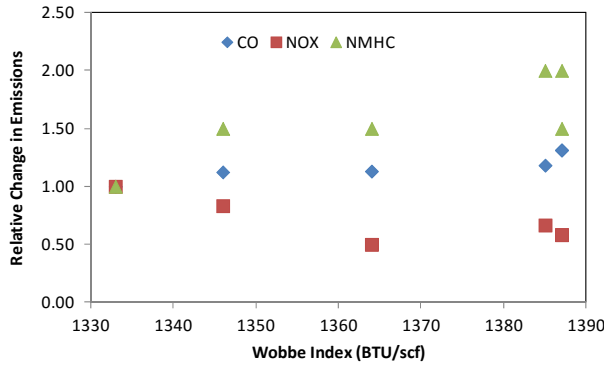
combustion engines. Only one source shows qualitatively the sensitivity of gas turbines to NG quality (GE, 2005). For the present study, large boilers from the utility and industrial sectors are assumed employ ultra-low NO_x burner technology. Because experimental data are unavailable, gas turbines are assumed to have the same emission sensitivity factor as low-NO_x burners. This is a gross assumption that introduces high uncertainty in the results. Experimental emission testing of gas turbines and engines would reduce this uncertainty.

3) Mobile Sources

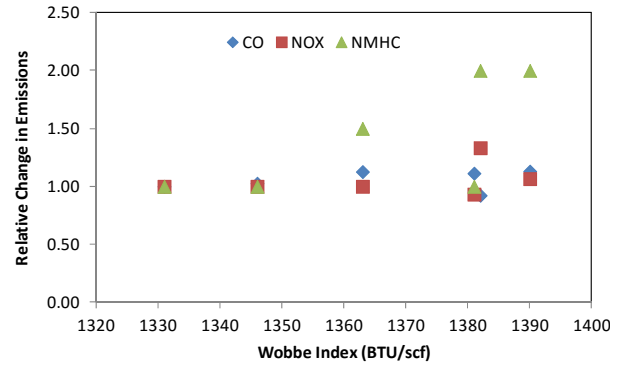
Experimental data on emissions from compressed natural gas (CNG) vehicles are also limited, but there are sufficient data to establish bounds on the impacts of natural gas composition on emissions. Emission factors for light-duty CNG vehicle were obtained from tests of a Honda Civic GX under two driving cycles (Crawford and Lyons, 2009), and for heavy-duty trucks, several models were tested with varying natural gas WI and Methane Number (MN) for heavy-duty trucks (Crawford and Lyons, 2010).

Figure 5 shows the changes in emissions of CO, NO_x and non-methane hydrocarbons (NMHC) due to changes in WI measured for a Honda Civic GX following two different driving cycles: Federal Test Procedure (FTP) and California Unified Cycle (CUC) (Crawford and Lyons, 2009). Emissions of CO and NMHC generally increase with increasing WI in both driving cycles. On the contrary, NO_x emissions sensitivity differs between cycles: as WI increase, NO_x emissions decrease for the FTP cycle, and increase for the CUC. For the modeling in this report, the maximum increases in pollutant emissions over the WI range 1330-1390 BTU/scf reported by Crawford and Lyons (2009) among the two cycles were used to determine the maximum impact of gas composition on vehicle emissions. These increases are 31%, 33% and 100% for CO, NO_x and NMHC, respectively, which are assumed for all light-duty vehicles.

Figure 6 presents the relative changes in pollutant emissions from heavy-duty CNG engines due to changes in MN and WI (Crawford and Lyons, 2010). There is a wide range of changes in pollutant emissions due to changing WI, including increases and decreases in emissions of CO, NO_x and NMHC. The maximum increases compared to a fuel with WI = 1335 BTU/scf were 28%, 22% and 67% for CO, NO_x and NMHC, respectively. As for light-duty vehicles, these maximum increases were used to in the TEMPLES model to determine the maximum impact of gas composition on emissions from heavy-duty trucks. Table 3 summarizes the emission sensitivity factors ($\Delta ef_{i,j,l}$) for light-duty and heavy-duty CNG vehicles used in this study.

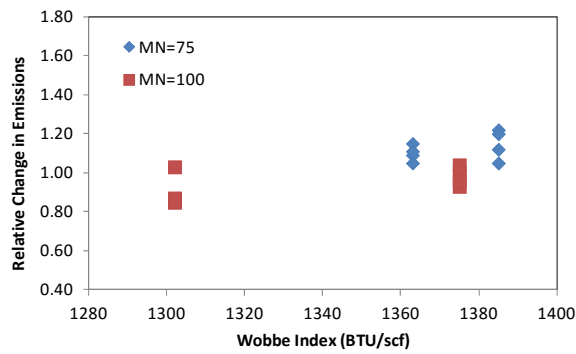


(a)

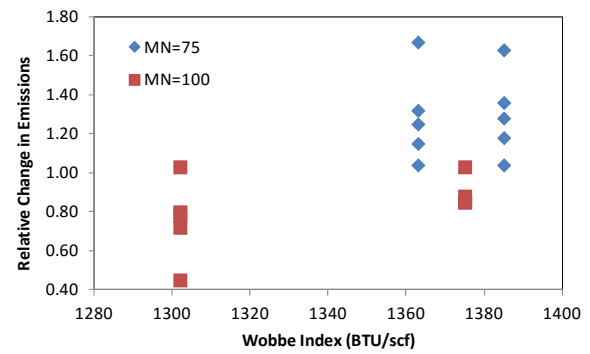


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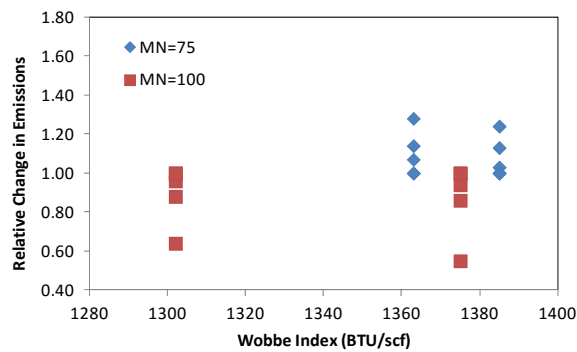
Figure 5 CNG passenger car emissions: (a) Federal Test Procedure (FTP), and (b) California Unified Cycle (CUC). (Data source: Crawford and Lyons, 2009).



(a)



(b)



(c)

Figure 6 CNG heavy-duty vehicle emissions due to changes in MN and WI. The changes are expressed relative to emissions using CNG with WI = 1335 BTU/scf for: (a) NO_x, (b) NMHC, and (c) CO. (Data source: Crawford and Lyons, 2010).

Table 3 Emission sensitivity factors ($\Delta ef_{i,j,l}$) for CNG vehicles.

Vehicle Type	Emission Sensitivity Factor (% per 50 BTU/scf increase in WI)		
	NOX	CO	NMHC
Light-duty CNG	33%	31%	100%
Heavy-duty CNG	22%	28%	67%

A statistical analysis of CNG mobile source emissions tests, similar to that conducted for residential sources, would provide more reliable estimates of natural gas composition impacts on vehicle emissions, but the current data are too limited to allow such an analysis. Using maximum emission changes demonstrates the use of TEMPLES for simulating natural gas composition effects on emissions from mobile sources and establishes maximum likely bounds on these impacts.

II.A.2 Natural Gas Tool Methodology

The overall process executed by the Custom Pre-Processor is to apply a multiplication factor to the baseline inventory (Base Emissions) to obtain the emissions for a particular NG case (Eq. 2). The multiplication factor depends on the natural gas composition (parameterized by a change in WI), emission sensitivity factors obtained from emission testing, and information on technology distribution to relate technologies tested with emission sources in the inventory.

$$\text{NG Case Emissions} = \text{Base Emissions} \times \text{Factor}(\Delta \text{WI, emission testing, tech distribution}) \quad (2)$$

The baseline emissions inventory is based on the 2005 National Emissions Inventory (NEI) developed by the US Environmental Protection Agency (U.S. EPA, 2011). The NEI contains area, on-road and off-road mobile, and point sources. Area and mobile sources are reported by Standard Classification Code (SCC) at a county level, and are allocated spatially at the necessary grid resolution using appropriate spatial surrogates. SCCs for area and mobile sources have ten digits that denote four levels of characterization in the format AA-BB-CCC-DDD. For area sources, level one (AA) denotes a process; level two (BB) is the major activity sector; level three (CCC) describes fuel use; and level four (DDD) denotes technology. For mobile sources, AA denotes mobile sources, BB denotes fuel, CCC denotes vehicle class and DDD denotes road type. SCCs for point sources have eight digits with four levels of characterization in the format A-BB-CCC-DD. For point sources, level one (A) denotes a type of process; level two (BB) denotes major activity sector; level three (CCC) denotes fuel use; and level four (DD) denotes technology.

Spatial surrogates are spatially-gridded weighting factors based on geographical and/or socio-economic factors to disaggregate emissions data with coarse resolution to a resolution that matches the emissions and air quality models. For example, residential, commercial and industrial sector sources of emissions are weighted using population density, commercial and industrial sector area distribution as respective surrogates. Emissions from mobile sources are allocated using the distribution of road miles as surrogate. Figure 7 presents the spatial distribution of population density, road distribution and commercial and industrial area distribution in California. Point sources are reported by SCC and by specific spatial coordinates, so spatial surrogates are not needed to allocate point source emissions. Table 4 through Table 7 present the sources by SCC that are related to natural gas combustion in the baseline inventory. Non-road mobile sources were not included in the analyses presented in this report due to lack of emission sensitivity data. The NEI does not include emissions data for NG vehicles, but that information is needed to evaluate the impacts of NG vehicle penetration in the future. ARB data on natural gas vehicle emissions will be incorporated to enable evaluation of the impact natural gas changes on mobile source emissions in the future.

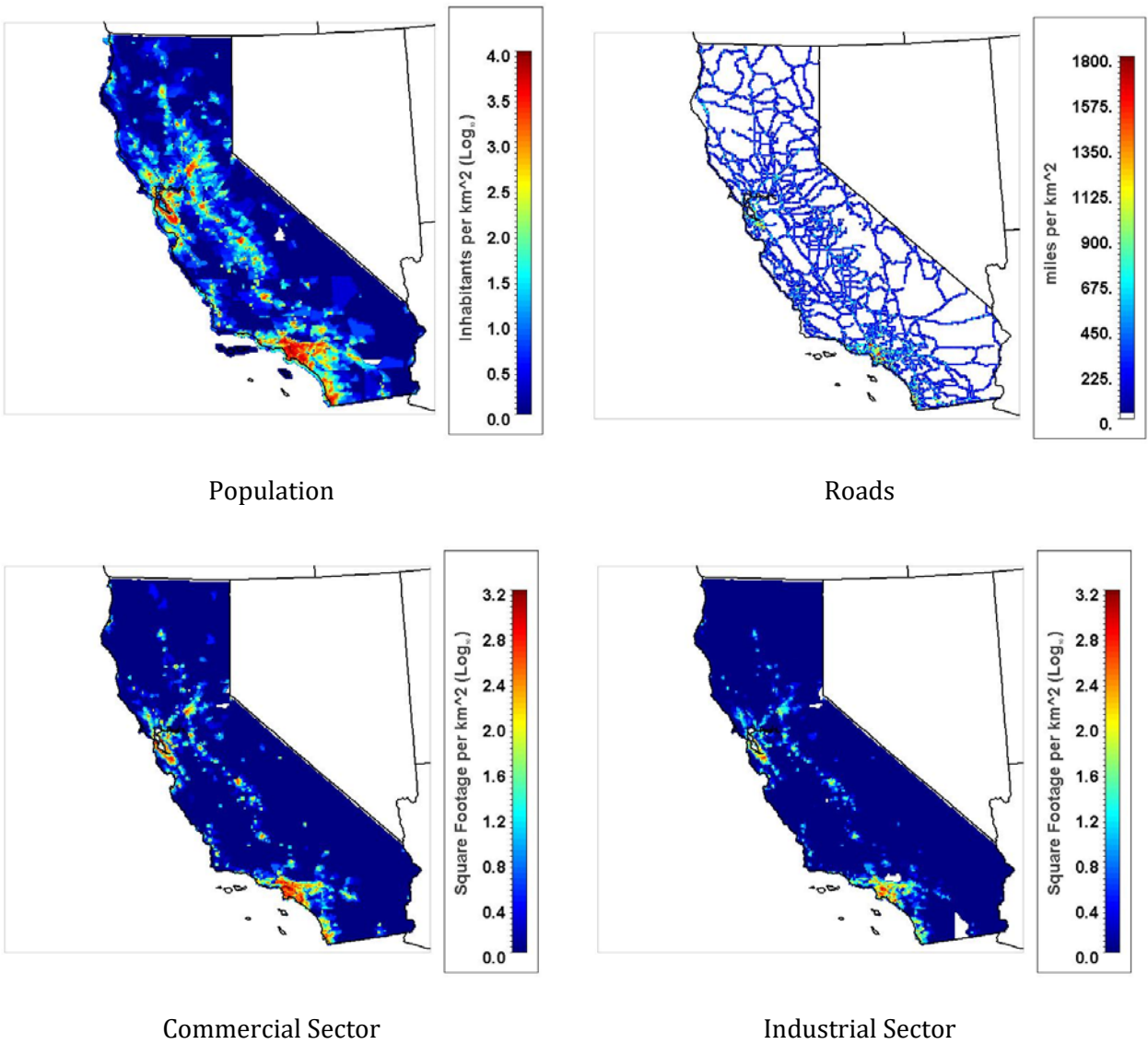


Figure 7 Examples of spatial surrogates for the entire State of California to allocate area emissions

Table 4 SCC descriptions for area sources.

SCC	SCC Level One	SCC Level Two	SCC Level Three	SCC Level Four
2101006000	Stationary Source Fuel Combustion	Electric Utility	Natural Gas	Total: Boilers and IC Engines
2102006000	Stationary Source Fuel Combustion	Industrial	Natural Gas	Total: Boilers and IC Engines
2102006002	Stationary Source Fuel Combustion	Industrial	Natural Gas	All IC Engine Types
2103006000	Stationary Source Fuel Combustion	Commercial/Institutional	Natural Gas	Total: Boilers and IC Engines
2104006000	Stationary Source Fuel Combustion	Residential	Natural Gas	Total: All Combustor Types
2104006010	Stationary Source Fuel Combustion	Residential Oil and Gas Exploration and Production	Natural Gas	Residential Furnaces
2310020000	Industrial Processes		Natural Gas	Total: All Processes

Table 5 SCC descriptions for non-road mobile sources.

SCC	SCC Level One	SCC Level Two	SCC Level Three	SCC Level Four
2268000000	Mobile Sources	CNG	Industrial Equipment	Sweepers/Scrubbers
2268003020	Mobile Sources	CNG	Construction and Mining Equipment	Rollers
2268006005	Mobile Sources	CNG	Agricultural Equipment	Agricultural Mowers
2268006020	Mobile Sources	CNG	Lawn and Garden Equipment	Lawn and Garden Tractors (Commercial)
2268008005	Mobile Sources	CNG	Agricultural Equipment	2-Wheel Tractors

Table 6 SCC descriptions for on-road mobile sources.

SCC	SCC Level One	SCC Level Two	SCC Level Three	SCC Level Four
2201001000	Mobile Sources	Highway Vehicles – Gasoline	Light-duty Gasoline Vehicles	All types
2201020000	Mobile Sources	Highway Vehicles – Gasoline	Light-duty Gasoline Trucks 1 & 2	All types
2201040000	Mobile Sources	Highway Vehicles – Gasoline	Light-duty Gasoline Trucks 3 & 4	All types
2201070000	Mobile Sources	Highway Vehicles – Gas	Heavy-duty Gasoline Vehicles	All types
2230060000	Mobile Sources	Highway Vehicles - Diesel	Light-duty Diesel Trucks	All types
2230070000	Mobile Sources	Highway Vehicles - Diesel	Heavy Duty Diesel Vehicles	All types

Table 7 SCC descriptions for point sources.

SCC	SCC Level One	SCC Level Two	SCC Level Three	SCC Level Four
10100601	External Combustion Boilers	Electric Generation	Natural Gas	Boilers : 100 Million Btu/hr except Tangential
10100602	External Combustion Boilers	Electric Generation	Natural Gas	Boilers < 100 Million Btu/hr except Tangential
10100604	External Combustion Boilers	Electric Generation	Natural Gas	Tangentially Fired Units
10200601	External Combustion Boilers	Industrial	Natural Gas	> 100 Million Btu/hr
10200602	External Combustion Boilers	Industrial	Natural Gas	10-100 Million Btu/hr
10200603	External Combustion Boilers	Industrial	Natural Gas	< 10 Million Btu/hr
10200604	External Combustion Boilers	Industrial	Natural Gas	Cogeneration
10300601	External Combustion Boilers	Commercial/Institutional	Natural Gas	> 100 Million Btu/hr
10300602	External Combustion Boilers	Commercial/Institutional	Natural Gas	10-100 Million Btu/hr
10300603	External Combustion Boilers	Commercial/Institutional	Natural Gas	< 10 Million Btu/hr
20100201	Internal Combustion Engines	Electric Generation	Natural Gas	Turbine
20100202	Internal Combustion Engines	Electric Generation	Natural Gas	Reciprocating
20100205	Internal Combustion Engines	Electric Generation	Natural Gas	Reciprocating: Crankcase Blowby
20200201	Internal Combustion Engines	Industrial	Natural Gas	Turbine
20200202	Internal Combustion Engines	Industrial	Natural Gas	Reciprocating
20200203	Internal Combustion Engines	Industrial	Natural Gas	Turbine: Cogeneration
20200204	Internal Combustion Engines	Industrial	Natural Gas	Reciprocating: Cogeneration
20200205	Internal Combustion Engines	Industrial	Natural Gas	Reciprocating: Crankcase Blowby
20200252	Internal Combustion Engines	Industrial	Natural Gas	2-cycle Lean Burn
20200253	Internal Combustion Engines	Industrial	Natural Gas	4-cycle Rich Burn
20200254	Internal Combustion Engines	Industrial	Natural Gas	4-cycle Lean Burn
20300201	Internal Combustion Engines	Commercial/Institutional	Natural Gas	Reciprocating
20300202	Internal Combustion Engines	Commercial/Institutional	Natural Gas	Turbine
20300203	Internal Combustion Engines	Commercial/Institutional	Natural Gas	Turbine: Cogeneration
20300204	Internal Combustion Engines	Commercial/Institutional	Natural Gas	Reciprocating: Cogeneration
39000602	Industrial Processes	In-process Fuel Use	Natural Gas	Cement Kiln/Dryer
39000603	Industrial Processes	In-process Fuel Use	Natural Gas	Lime Kiln
39000699	Industrial Processes	In-process Fuel Use	Natural Gas	General

For the calculation of the multiplication factor, changes in WI are based on the assumption that California's average NG has a WI of 1335 BTU/scf, and are defined at a county level. Using WI to describe a new fuel source is a simplification of what is likely to be a much more complex variation in fuel properties. However, WI is a commonly used metric for relating emission factors in natural gas burners to natural gas quality and is therefore a natural fit for this model (Martinez *et al.*, 2013; Southern California Gas, 2004, 2006a, 2006b)). The methodology to determine the multiplication factor, which uses the emission testing data presented in section II.A.1 and technology distribution factors that establish a relation between NG specific technologies and SCC codes is presented below in four steps. Terms used in the methodology are defined as follows:

Symbol	Definition	Units
i	Appliance/technology evaluated experimentally	- *
j	Type of source: area, mobile, point	-
k	Standard Classification Code	-
l	Pollutant emitted: NO _x , CO, SO _x , VOC, PM	-
m	Location (i.e., county)	-
$ef_{i,j,l}$	Baseline emission factor for technology i , in source category j , for pollutant l	ng/J or - **
$\Delta ef_{i,j,l}$	Emission sensitivity factor by technology i due to 50 BTU/scf increase in WI	ng/J or % **
$EF_{j,k,l}$	Baseline emission factor for SCC k , in source category j , for pollutant l	ng/J or - **
$\Delta EF_{j,k,l}$	Increase in emission factor by SCC k due to 50 BTU/scf increase in WI	ng/J or % **
$f_{i,j,k}$	Technology distribution factor between technology i , and SCC k , by source type j	-
ΔWI_m	Increment in WI from baseline at location m	BTU/scf
$I_{j,k,l,m}$	Impact in emissions – multiplication factor – per source category j , SCC k , pollutant l and at location m	-
$E_{j,k,l,m}$	Baseline emissions per source category j , SCC k , pollutant l and at location m	tpd
$uE_{j,k,l,m}$	Updated emissions per source category j , SCC k , pollutant l and at location m	tpd
X_{NG}	Fraction of vehicles converted to NG	-
(EF_{NG}/EF_{CV})	NG to conventional vehicle ratio of emission factors for pollutant l	-

*- represents dimensionless

**For commercial, industrial and mobile sources emission sensitivity factors are expressed as % relative to baseline factors, and baseline factors are not needed for calculations

STEP 1: Calculate values of $EF_{j,k,l}$, the baseline emission factors for each SCC and type of source.

Prior to calculating the increment in emissions due to changes in WI, baseline emission factors, $EF_{j,k,l}$, for each type of source j , SCC code k , and pollutant l , need to be estimated using Equation 3. Each activity sector k denoted by an SCC may include a variety of technologies and/or appliances i . For instance, SCC 2104006000 corresponds to residential natural gas combustion, which can include cooking and water heating. For cooking, emissions from several types of burners have been measured, and all of them contribute to the total emissions for that SCC. Hence, there is the need for technology distribution factors, $f_{i,j,k}$, to define the distribution of technology i , in each source type j and within each SCC code k . The $f_{i,j,k}$ values used in this study for area and on-road mobile sources are presented in Table 8, and those for point sources are given in Table 9. There are some technology surveys that report the technology mix in use for some appliances (KEMA, 2010; Klug et al. 2011), but data are generally scarce and assumptions are required to complete the entire matrix of $f_{i,j,k}$ values. The baseline emission factors, $ef_{i,j,l}$, for residential appliances are presented in Table 1. The baseline emission factors for the commercial, industrial and mobile sources are assumed to be 1, because the emission sensitivity factors, $\Delta ef_{i,j,l}$, are expressed in relative terms with respect to $ef_{i,j,l}$.

$$EF_{j,k,l} = \sum_i f_{i,j,k} \cdot ef_{i,j,l} \quad (3)$$

STEP2: Calculate values of $\Delta EF_{j,k,l}$, incremental emission factors for each SCC and type of source.

Incremental emission factors, $\Delta EF_{j,k,l}$, for each type of source j , SCC code k , and pollutant l , and for a 50 BTU/scf increase in WI are calculated by Equation 4, using the same technology distribution factors $f_{i,j,k}$ that define a technology mix in a particular SCC and the emission sensitivity factors from reported experimental measurements, $\Delta ef_{i,j,l}$ (presented in Table 1-Table 3).

$$\Delta EF_{j,k,l} = \sum_i f_{i,j,k} \cdot \Delta ef_{i,j,l} \quad (4)$$

STEP3: Calculate values of $I_{j,k,l}$, the spatially resolved relative increase in emissions due to changes in WI.

The multiplication factors, $I_{j,k,l,m}$, which is applied to each source category j , SCC code k , pollutant l and at location m , are calculated using Equation 5. The change in emissions due to a change in WI is assumed linear over the expected WI range for each technology type. Because $\Delta ef_{i,j,l}$ and $\Delta EF_{j,k,l}$ values are expressed as a change in emissions per 50 BTU/scf increment in WI, the increase in emissions is proportional to the WI change, ΔWI_m , that occurs in location m (county), divided by 50 BTU/scf.

$$I_{j,k,l,m} = 1 + \frac{\Delta WI_m}{50} \cdot \frac{\Delta EF_{j,k,l}}{EF_{j,k,l}} \quad (5)$$

STEP4: Calculate values of $uE_{j,k,l,m}$, the spatially resolved updated emissions for the defined scenario.

The updated emissions for a particular NG Case are calculated using Equation 6. The baseline emissions are multiplied by the $I_{j,k,l,m}$ values to perturb baseline emissions and obtain the emissions for a particular scenario for type of source j , SCC code k , pollutant l and location m .

$$uE_{j,k,l,m} = I_{j,k,l,m} \cdot E_{j,k,l,m} \quad (6)$$

For vehicle scenarios, the model assumes that only a fraction of vehicles, X_{NG} , is converted to NG vehicles. Hence, the multiplication factors $I_{j,k,l,m}$ are applied only to the fraction of NG vehicles. In addition, baseline emissions from NG vehicles differ from baseline emissions from conventional vehicles. Hence, a correction factor must be applied to the fraction X_{NG} of vehicles, $\left(\frac{EF_{NG}}{EF_{CV}}\right)_l$. The remaining $(1 - X_{NG})$ fraction of vehicles is not altered by the multiplication factors, $I_{j,k,l,m}$. As a result, the vehicle emissions are calculated using Equation 7.

$$uE_{j,k,l,m} = (1 - X_{NG}) \cdot E_{j,k,l,m} + X_{NG} \cdot \left(\frac{EF_{NG}}{EF_{CV}}\right)_l \cdot I_{j,k,l,m} \cdot E_{j,k,l,m} \quad (7)$$

Table 8: Technology distribution factors ($f_{ij,l}$) for area and on-road mobile sources.

SCC	Furnace	Storage Water Heater	Tank-less Water Heater	Cook-top	Oven Burner	Broiler Burner	Low-NO _x Burner	Ultralow-NO _x Burner	Light Duty CNG	Heavy-Duty CNG
2101006000							1			
2102006000							1			
2102006002							1			
2103006000	0.3	0.3					0.4			
2104006000		0.35	0.15	0.4	0.08	0.02				
2104006010	1									
2310020000							1			
2101006000							1			
2201001000									1	
2201020000									1	
2201040000									1	
2201070000										1
2230060000										1
2230070000										1

Table 9 Technology distribution factors ($f_{ij,l}$) for point sources.

SCC	Low-NO _x Burner	Ultralow- NO _x Burner
10100601		1
10200601		1
10300601	1	
20100201	1	
20200201	1	
20300201	1	
39000602	1	

II.B Air Quality Modeling

Tropospheric ozone is a product of photochemistry between NO_x and volatile organic compounds (VOCs) in the ambient atmosphere in the presence of sunlight. In California, NO_x and VOCs are mostly emitted from anthropogenic sources such as on-road and off-road vehicles, power plants and industrial operations, although there are significant biogenic sources of VOCs (CARB, 2009b). Ozone concentrations depend on spatial and temporal profiles of precursor emissions, meteorological conditions, transport of precursors and reaction products through, and removal processes such as deposition and chemical reaction. Comprehensive models that incorporate all these physical and chemical processes in detail are widely used to understand and characterize ozone formation on regional scales. These air quality models numerically solve a series of atmospheric chemistry, diffusion, and advection equations in order to determine ambient concentrations of pollutants within control volumes over a given geographic region.

Most models employ an Eulerian representation (i.e., one that considers changes as they occur at a fixed location in the fluid, usually called a cell or control volume) of physical quantities on a three-dimensional computational grid. The atmospheric advective diffusion equation for species m in a given control volume is:

$$\frac{\partial Q_m^k}{\partial t} = -\nabla \cdot (uQ_m^k) + \nabla \cdot (K\nabla Q_m^k) + \left(\frac{Q_m^k}{\partial t} \right)_{sources / sinks} + \left(\frac{Q_m^k}{\partial t} \right)_{aerosol} + \left(\frac{Q_m^k}{\partial t} \right)_{chemistry} \quad (8)$$

where t is time, k is phase – gas or aerosol, u is wind velocity and K is the coefficient of eddy diffusivity tensor that parameterizes turbulent diffusion.

The above equation is numerically integrated in time to obtain the concentration, Q , of each species m in phase k (gas phase or aerosol phase), over a series of discrete time steps in each of the spatially distributed discrete cells of the air quality model. Each term on the right side of the advective diffusion equation represents a major process in the atmosphere. From left to right these are: (1) advective transport due to wind, (2) turbulent diffusion due to atmospheric stability/instability, (3) emission (sources) and deposition (sinks), (4) mass transfer between gas and aerosol phases, and (5) chemical reaction.

The outputs from air quality models are spatially and temporally resolved concentrations of pollutant species within control volumes over a geographic region. To minimize the effects of initial conditions, air quality simulations are performed over multiple days and results from the first few days are not included in the analysis.

The CMAQ model (Byun and Ching, 1999) is a comprehensive air quality modeling system developed by the United States Environmental Protection Agency (US EPA) and is used in many regulatory air quality applications such as studying tropospheric ozone, particulate matter, acid deposition and visibility (Appel *et al.* 2008, 2010; Foley *et al.* 2010). The chemical mechanism used in CMAQ is the CB05 (Sarwar *et al.*, 2008), which includes the photochemical formation of ozone, oxidation of volatile organic compounds and formation of organic aerosol precursors. The advection model in CMAQ is based on the Yamartino-Blackman Cubic Scheme (Yamartino, 1993) and vertical turbulent mixing is based on K-theory (Chang *et al.*, 1987, and Hass *et al.*, 1991). For the simulations presented in this report, the spatial resolution of control volumes is $4\text{km} \times 4\text{km}$ over the entire state, and a vertical height of 10,000 meters above ground, with 30 layers of variable height based on pressure distribution. Meteorological input data for CMAQ was obtained from the Advanced Research Weather Research and Forecasting Model, WRF-ARW (Skamarock *et al.* 2005). The National Centers for Environmental Prediction (NCEP) Final Operational Global Analysis $1^\circ \times 1^\circ$ grid data (NCEP, 2005) were used for WRF-ARW initial and boundary conditions.

III Simulated Scenarios

This report demonstrates some modeling capabilities of the TEMPLES/CMAQ software developed at UC Irvine to address questions about the impacts of changing natural gas quality on emissions from natural gas equipment and engines. Six sample cases are simulated to provide an overview of the TEMPLES/CMAQ capabilities and to illustrate likely impacts of changing natural gas quality on statewide emissions and air quality. In addition, certain cases demonstrate the model's sensitivity to input parameters. These cases were developed to simulate real world and to provide ARB with useful preliminary results for evaluating the impacts of natural gas compositions on air quality.

Table 10 Simulation scenarios.

Scenarios	Description
<i>Base Cases</i>	
Summer Baseline	Baseline emissions from the 2005 National Emissions Inventory for a week in July
Winter Baseline	Baseline emissions from the 2005 National Emissions Inventory for a week in December
CNG Base Case	Baseline emissions from the 2005 National Emissions Inventory for a week in July, assuming a CNG vehicle penetration of 5%
<i>Study Cases</i>	
Case A	Summer-time natural gas quality shift of $\Delta WI = +50$ BTU/scf, with respect to Summer Baseline
Case B	Summer-time natural gas quality shift of $\Delta WI = +50$ BTU/scf with maximum burner sensitivity, with respect to Summer Baseline
Case C	Impact of natural gas quality shift of $\Delta WI = +50$ BTU/scf on large electricity generation point sources only, with respect to Summer Baseline
Case D	Impact of LNG importation to San Diego County, with respect to Summer Baseline
Case E	Winter-time natural gas quality shift of $\Delta WI = +50$ BTU/scf, with respect to Winter Baseline
Case F	Summer-time natural gas quality shift of $\Delta WI = +50$ BTU/scf for CNG vehicles only, with respect to CNG Base Case

Base Cases

Summer Baseline:

The Summer Baseline is the 2005 National Emissions Inventory (NEI) developed by the U.S. EPA, composed of data collected by ARB and local air districts. For this case, the WI for all of the NG used in the state is 1335 BTU/scf. This case assumes no changes in natural gas composition and is the reference emission inventory for a summer episode. . Temporal profiles for some NG combustion sources, such as space heating, vary throughout the year because of seasonal variability in usage. The SMOKE model incorporates typical temporal profiles for all emission sources so that those seasonal variations are reflected in the spatially-resolved emissions. This particular case represents a typical week in July 2005.

Winter Baseline:

The Winter Baseline case is the 2005 National Emissions Inventory (NEI) developed by the US EPA for a typical week in December 2005. As for the Summer Baseline, this case a 1335 BTU/scf WI for all NG used in the state and is the reference emission inventory for a winter episode.

CNG Base Case:

The CNG Base Case is a variation of the Summer Baseline case where 5% of light and heavy duty vehicles are replaced by CNG vehicles. The rest of inputs are exactly the same as the Summer Baseline case. This base case assumes that the WI for all of the NG used in the state is 1335 BTU/scf. The CNG vehicle penetration of 5% was chosen arbitrarily to demonstrate TEMPLES capabilities; any CNG vehicle penetration level may be modeled.

A 2006 survey determined that there were 20,419 light-duty CNG vehicles in California (Gas Technology Institute, 2006), approximately 0.16% of the 13 million passenger cars in the state (ARB, 2009). That study also estimated that there were 5,489 medium-duty and 3,857 heavy-duty CNG vehicles in the state. A separate study focused on Southern California determined that there were 5,780 heavy-duty CNG vehicles altogether in Los Angeles, Orange, Riverside and San Bernardino counties, which corresponds to nearly 3% of the medium-heavy duty and heavy-heavy duty vehicles on the road in 2008 in those counties (ARB, 2009). Current penetration of CNG vehicles is significantly lower than 5%, especially for light-duty vehicles, but decreasing NG prices could increase CNG vehicle

sales. Hence, a penetration of 5% provides an upper bound for evaluating vehicle emissions impacts from changing natural gas quality.

Study Cases

Case A: Summer-Time Natural Gas Quality Shift of $\Delta WI = +50$ BTU/scf:

This case is identical to the Summer Baseline case, but applies an increase in WI from 1335 to 1385 BTU/scf for natural gas used throughout the state. All natural gas combustion emission sources burn the higher WI fuel. For all technologies, a median or best estimate value for the changes in emission rates for all species and burner technologies are assumed. Thus, for residential burners, the Best Engineering Estimates for emission sensitivity factors from Table 1 are used. For commercial and industrial sources, emission sensitivity factors from Table 2 are used. Effects of changing WI on emissions from CNG vehicles are omitted in this scenario.

Case B: Summer-Time Natural Gas Quality Shift of $\Delta WI = +50$ BTU/scf with Maximum Burner Sensitivity

Similarly to Case A, this case uses the Summer Baseline, and assumes a WI increase from 1335 to 1385 BTU/scf for natural gas used throughout the state. The only difference with Case A is the emission factor assumed for residential appliances; the Maximum Likely Increase from Table 1 is used here as opposed to the Best Engineering Estimate used for Case A. All stationary natural gas combustion emission sources are assumed to burn the higher WI fuel. Effects of changing WI on emissions from CNG vehicles are also omitted in this scenario.

Case C: Impact of Natural Gas Quality Shift of $\Delta WI = +50$ BTU/scf on Large Electricity Generation Point Sources

This case evaluates the impacts of increasing Wobbe Index on emissions from large power generation only. The reference case for this scenario is the Summer Baseline inventory. Emissions from electric power generation contribute 2% of total statewide NO_x emissions, and those emissions are point sources released from stacks. Based on the state emissions inventory for 2005, 61% of the point source NO_x emissions from natural gas combustion for power generation are from large gas turbines, 32% are from large boilers, and the remaining 7% are from small boilers and engines. Nearly 5% of the installed capacity in state consists of peaker plants, which are typically single cycle gas turbines that accommodate rapid fluctuations in power demand. Emissions of peaker plants are typically higher than base-load plants, and changes in the gas composition could impact emissions from these turbines. This case assumes that only large power generators experience NG with a higher WI, which is not a realistic scenario because power generators

combust the same natural gas as other users. This hypothetical scenario illustrates the contribution to emission changes from power generation alone should natural gas composition change, and it demonstrates the ability of TEMPLES to evaluate isolated impacts from specific emission sectors.

Case D: Liquefied Natural Gas Importation to San Diego County

This case evaluates the emissions and air quality impacts in San Diego County when a portion of the natural gas supply is imported liquefied natural gas (LNG) from Mexico. The Energy Costa Azul (ECA) liquefied natural gas (LNG) terminal in Baja California, Mexico has the capacity to import approximately one billion cubic feet per day of gasified LNG from overseas, and a portion of this can be transmitted into California. Such imports to California have occurred briefly in the past, but due to the widespread extraction of shale gas in the US, no LNG is currently imported into California. While that is the current reality, energy markets regularly shift, and future LNG imports to California remain a possibility. Because of its proximity to the ECA terminal and the natural gas flows in transmission pipelines, San Diego County is likely to consume nearly all LNG imported to California. In addition to evaluating the air quality impacts of potential LNG imports, this case also illustrates the ability of TEMPLES to analyze the contribution of local emissions to air quality in neighboring areas (i.e., emissions from San Diego County impacting air quality in Los Angeles County).

This scenario uses all of the same input parameters as Case B, but the WI increase is assumed to only occur in San Diego County. By comparing this case with Case B one can determine the degree to which individual counties can be considered to be isolated from the remainder of the domain, and it illustrates the relative importance of close-range and long-range emissions sources.

Case E: Winter-Time Natural Gas Quality Shift of $\Delta WI = +50$ BTU/scf

This case uses the same inputs as the Winter Baseline, but with an increase in WI from 1335 to 1385 BTU/scf for natural gas used throughout the state. Two major changes in the input files generated by the pre-processors that support TEMPLES/CMAQ are implemented compared to the Winter Baseline case. First, meteorological conditions affect biogenic and evaporative emissions. Winter conditions tend to produce lower biogenic and evaporative emissions due to lower temperatures. Second, human activities, like space and water heating, experience seasonal variations with higher winter-time emissions that are accounted for by SMOKE.

Case F: Increase in On-Road Natural Gas Vehicles

This scenario studies the effect of changing WI on the emissions from only CNG vehicles. The reference for this simulation is the CNG Base Case. Natural gas vehicles are among the alternative fuel vehicle options included in ARB initiatives to reduce mobile source emissions. By comparison to the CNG Base Case, this case evaluates the statewide emissions and air quality impacts of increasing WI by 50 BTU/scf only in the NG used to fuel the CNG vehicles introduced in the CNG Base Case (5% penetration of CNG vehicles into the statewide fleet for both light-duty and heavy-duty vehicles).

IV Impacts of Gas Composition on Emissions

This section presents tables of absolute emissions for the Base Cases and the Study Cases. Pollutant emissions for all scenarios are disaggregated by the Source Classification Codes (SCC), which indicate specific emission. Table 4, Table 6 and Table 7 present SCCs and their corresponding description for area, mobile and point sources considered in the modeling scenarios. For stationary sources – area and point sources – these emissions tables focus on NO_x. Emission sensitivity factors for CO were available for residential appliances, so the values of CO emissions are also reported for completeness. However, since CO has low reactivity and does not significantly impact ozone formation, discussion of the impacts of changing NG composition are centered on the analysis of NO_x emissions. For mobile sources considered in Scenario F, discussion of VOC emissions is included because VOC emission sensitivity factors were available.

Table 11 presents the total natural gas-related emissions from stationary sources for the Summer Baseline and the Winter Baseline cases. The three largest contributors to total NO_x emissions in the summer are industrial natural gas combustion from boilers and engines (SCC 2102006000 and 2102006002) and commercial sector natural gas combustion (2103006000), with NO_x emissions ranging from 52, to 24 short tons per day (tpd). It is important to note that these sources are assumed to use low-NO_x burners which are very sensitive to changes in WI. Other large sources of NO_x emissions include oil and gas operations (2310020000) with 17 tpd, boilers (10100601) with 9 tpd, and gas turbines (20100201) for electricity production with 21 tpd.

The largest differences in emissions between summer and winter are due to the higher emissions from residential and commercial combustion for water and space heating during wintertime, the shaded entries in Table 11. NO_x emissions from SCC 2103006000 – commercial and institutional boilers and engines – and from 2104006000 and 2104006010 – residential NG combustion – increase by 32, 71 and 62 tpd, respectively, from Summer Baseline to Winter Baseline. CO emissions also experienced increases in the same SCC designations from summer to winter.

Table 11 2005 Statewide stationary natural gas combustion emissions (tpd)

SCC	Summer Baseline		Winter Baseline		Difference Winter - Summer	
	CO	NO _x	CO	NO _x	CO	NO _x
2101006000	12.33	6.61	12.33	6.61	0.00	0.00
2102006000	14.49	52.52	14.49	52.52	0.00	0.00
2102006002	15.71	40.49	15.71	40.49	0.00	0.00
2103006000	11.81	24.12	27.63	56.44	15.82	32.32
2104006000	0.89	1.93	33.84	73.19	32.95	71.27
2104006010	0.71	1.68	26.97	63.83	26.26	62.15
2310020000	7.73	16.55	7.73	16.55	0.00	0.00
10100601	41.43	8.73	38.92	8.67	-2.51	-0.06
10100602	0.09	0.20	0.10	0.21	0.01	0.02
10100604	0.00	0.01	0.00	0.00	0.00	0.00
10200601	23.16	2.75	23.14	2.79	-0.02	0.04
10200602	3.49	4.03	3.53	4.10	0.04	0.07
10200603	1.06	2.05	1.24	2.39	0.18	0.34
10200604	0.08	0.20	0.08	0.21	0.00	0.01
10300601	0.92	0.30	0.94	0.31	0.02	0.01
10300602	1.42	1.35	1.73	1.58	0.31	0.24
10300603	1.09	1.28	1.24	1.46	0.15	0.18
20100201	16.82	21.38	16.78	21.81	-0.04	0.43
20100202	2.07	1.30	2.07	1.31	0.00	0.00
20100205	0.00	0.00	0.00	0.00	0.00	0.00
20200201	2.45	4.11	2.42	4.09	-0.02	-0.02
20200202	14.31	10.32	14.61	10.56	0.30	0.25
20200203	2.24	5.43	2.17	5.38	-0.06	-0.05
20200204	0.43	0.35	0.44	0.35	0.00	0.00
20200205	0.00	0.00	0.00	0.00	0.00	0.00
20200252	0.07	0.33	0.07	0.33	0.00	0.00
20200253	0.83	0.84	0.83	0.84	0.00	0.00
20200254	0.06	0.32	0.06	0.32	0.00	0.00
20300201	5.12	1.41	4.88	1.35	-0.24	-0.07
20300202	0.54	1.48	0.55	1.55	0.01	0.07
20300203	4.13	5.65	4.13	5.76	0.00	0.11
20300204	0.21	0.16	0.21	0.16	0.00	0.00
39000602	0.07	0.13	0.07	0.13	0.00	0.00
39000603	0.09	0.22	0.09	0.22	0.00	0.00
39000699	1.20	4.33	1.20	4.33	0.00	0.00
Total	187.03	222.57	260.19	389.84	73.17	167.28

Table 12 presents the total natural gas-related emissions and Table 13 presents the emissions increases for modeling cases A, B, C and D. Emissions increases are with respect to the Summer Baseline case and expressed in tons per day. Negative values represent a decrease in emissions from Summer Baseline. Cases A and B have the highest increases in emissions. The only difference between Cases A and B is the emissions sensitivity factor assumed in the residential sector. However, since the emissions increases are dominated by area sources in the industrial sector (SCCs 2102006000 and 2102006002) and commercial/institutional sector (2103006000), the NO_x emissions increase for Cases A and B with respect to Summer Baseline are very similar: Case A increased by 63 tpd and Case B increased by 64 tpd. The difference between using the “Best Engineering Estimate” and “Maximum Likely Increase” emission sensitivity factor for residential sources generates a difference that totals 1 tpd in NO_x emissions over the entire state of California. Total 2005 statewide NO_x emissions were approximately 3,500 tpd (ARB, 2009b), so the 63-64 tpd increase for Cases A and B reflect a 1.8% increase compared to the Summer Baseline.

Case C models the impacts of WI changes on the emissions from the electricity generation sector alone: SCC 10100601 for large boilers and SCC 20100201 for turbines. Boilers were assumed to have ultra-low NO_x burners, whereas turbines were assumed to use low-NO_x burners (see discussion in Section II.A.1). Results for this scenario show an increase of 9.86 tpd (0.3%) in NO_x emissions with respect to the Summer Baseline. Case C was modeled assuming that all large turbines use low NO_x technology, which experience a 40% increase in NO_x emissions over the 50 Btu/scf WI change under consideration. However, large turbines typically include dynamic emission controls that compensate for changes in gas composition. As a result, the emission increases for Case C are likely to represent a worst-case emissions scenario for large turbines responding to a change in gas composition.

Case D illustrates the potential impacts of imported LNG to San Diego County. The total NO_x emissions in San Diego county increase by 2.35 tpd compared to the Summer Baseline case. This case is simply the same as Case B, but with increases in emissions only affecting San Diego County.

Table 12 Statewide emissions of CO and NO_x from all natural gas-related sources for Summer Baseline, and Cases A, B, C and D by SCC (tpd)

SCC	Summer Baseline		Case A		Case B		Case C		Case D	
	CO	NO _x	CO	NO _x	CO	NO _x	CO	NO _x	CO	NO _x
2101006000	12.33	6.61	12.33	9.26	12.33	9.26	12.33	6.61	12.33	7.67
2102006000	14.49	52.52	14.49	73.53	14.49	73.53	14.49	52.52	14.49	52.54
2102006002	15.71	40.49	15.71	56.68	15.71	56.68	15.71	40.49	15.71	40.57
2103006000	11.81	24.12	18.33	28.16	47.32	28.54	11.81	24.12	31.46	24.23
2104006000	0.89	1.93	0.84	1.97	1.00	2.03	0.89	1.93	0.89	1.93
2104006010	0.71	1.68	1.22	1.71	3.28	1.78	0.71	1.68	0.78	1.68
2310020000	7.73	16.55	7.73	23.17	7.73	23.17	7.73	16.55	7.73	16.55
10100601	41.43	8.73	41.43	10.04	41.43	10.04	41.43	10.04	41.43	8.90
10100602	0.09	0.20	0.09	0.20	0.09	0.20	0.09	0.20	0.09	0.20
10100604	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01
10200601	23.16	2.75	23.16	3.16	23.16	3.16	23.16	2.75	23.16	2.88
10200602	3.49	4.03	3.49	4.03	3.49	4.03	3.49	4.03	3.49	4.03
10200603	1.06	2.05	1.06	2.05	1.06	2.05	1.06	2.05	1.06	2.05
10200604	0.08	0.20	0.08	0.20	0.08	0.20	0.08	0.20	0.08	0.20
10300601	0.92	0.30	0.92	0.43	0.92	0.43	0.92	0.30	0.92	0.30
10300602	1.42	1.35	1.42	1.35	1.42	1.35	1.42	1.35	1.42	1.35
10300603	1.09	1.28	1.09	1.28	1.09	1.28	1.09	1.28	1.09	1.28
20100201	16.82	21.38	16.82	29.94	16.82	29.94	16.82	29.94	16.82	22.10
20100202	2.07	1.30	2.07	1.30	2.07	1.30	2.07	1.30	2.07	1.30
20100205	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200201	2.45	4.11	2.45	5.75	2.45	5.75	2.45	4.11	2.45	4.16
20200202	14.31	10.32	14.31	10.32	14.31	10.32	14.31	10.32	14.31	10.32
20200203	2.24	5.43	2.24	5.43	2.24	5.43	2.24	5.43	2.24	5.43
20200204	0.43	0.35	0.43	0.35	0.43	0.35	0.43	0.35	0.43	0.35
20200205	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200252	0.07	0.33	0.07	0.33	0.07	0.33	0.07	0.33	0.07	0.33
20200253	0.83	0.84	0.83	0.84	0.83	0.84	0.83	0.84	0.83	0.84
20200254	0.06	0.32	0.06	0.32	0.06	0.32	0.06	0.32	0.06	0.32
20300201	5.12	1.41	5.12	1.98	5.12	1.98	5.12	1.41	5.12	1.41
20300202	0.54	1.48	0.54	1.48	0.54	1.48	0.54	1.48	0.54	1.48
20300203	4.13	5.65	4.13	5.65	4.13	5.65	4.13	5.65	4.13	5.65
20300204	0.21	0.16	0.21	0.16	0.21	0.16	0.21	0.16	0.21	0.16
39000602	0.07	0.13	0.07	0.18	0.07	0.18	0.07	0.13	0.07	0.13
39000603	0.09	0.22	0.09	0.22	0.09	0.22	0.09	0.22	0.09	0.22
39000699	1.20	4.33	1.20	4.33	1.20	4.33	1.20	4.33	1.20	4.33
Total	187.03	222.57	194.01	285.80	225.22	286.31	187.03	232.43	206.75	224.92

Table 13 Statewide emissions increases of CO and NO_x of all natural gas-related sources for Cases A, B, C and D by SCC (tpd)

SCC	Case A		Case B		Case C		Case D	
	CO	NO _x	CO	NO _x	CO	NO _x	CO	NO _x
2101006000	0.00	2.65	0.00	2.65	0.00	0.00	0.00	1.06
2102006000	0.00	21.01	0.00	21.01	0.00	0.00	0.00	0.02
2102006002	0.00	16.20	0.00	16.20	0.00	0.00	0.00	0.08
2103006000	6.52	4.04	35.51	4.42	0.00	0.00	19.65	0.11
2104006000	-0.05	0.04	0.11	0.10	0.00	0.00	0.00	0.00
2104006010	0.51	0.03	2.57	0.10	0.00	0.00	0.07	0.00
2310020000	0.00	6.62	0.00	6.62	0.00	0.00	0.00	0.00
10100601	0.00	1.31	0.00	1.31	0.00	1.31	0.00	0.17
10100602	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10100604	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10200601	0.00	0.41	0.00	0.41	0.00	0.00	0.00	0.13
10200602	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10200603	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10200604	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10300601	0.00	0.12	0.00	0.12	0.00	0.00	0.00	0.00
10300602	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10300603	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20100201	0.00	8.55	0.00	8.55	0.00	8.55	0.00	0.72
20100202	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20100205	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200201	0.00	1.64	0.00	1.64	0.00	0.00	0.00	0.05
20200202	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200203	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200204	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200205	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200252	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200253	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20200254	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20300201	0.00	0.57	0.00	0.57	0.00	0.00	0.00	0.00
20300202	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20300203	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
20300204	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
39000602	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00
39000603	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
39000699	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total	6.98	63.24	38.20	63.74	0.00	9.86	19.73	2.35

Table 14 presents statewide CO and NO_x emissions by SCC for all NG-related sources for the Winter Baseline case and for Case E. Case E and Case B are similar, they both assume the same emissions sensitivity factors, but Case E evaluates changes from the Winter Baseline and Case B is a perturbation from the Summer Baseline. For Case E, the increase in statewide NO_x emissions from the Winter Baseline case is 71 tpd, whereas Case B produced an increase of 64 tpd. This 7 tpd statewide difference is due to the higher NO_x emissions from residential and commercial combustion for water and space heating during

wintertime with respect to summer emissions. Total statewide winter 2005 NO_x emissions were estimated to be 3,600 tpd (ARB, 2009b), so NO_x emissions increase by approximately 2% with respect to the Winter Baseline in Case E.

Table 15 through Table 17 summarizes CO and NO_x emissions and emission increments for each county in California for the Summer Baseline and Winter Baseline, and for Cases A through E.

Table 14 Statewide emissions of CO and NO_x from all natural gas-related sources for Winter Baseline and Case E (tpd)

SCC	Winter Baseline		Case E		Difference Case E – Base	
	CO	NO _x	CO	NO _x	CO	NO _x
2101006000	12.33	6.61	12.33	9.26	0.00	2.65
2102006000	14.49	52.52	14.49	73.53	0.00	21.01
2102006002	15.71	40.49	15.71	56.68	0.00	16.20
2103006000	27.63	56.44	42.89	65.90	15.27	9.46
2104006000	33.84	73.19	31.88	74.69	-1.97	1.50
2104006010	26.97	63.83	46.31	65.02	19.34	1.19
2310020000	7.73	16.55	7.73	23.17	0.00	6.62
10100601	38.92	8.67	38.92	9.97	0.00	1.30
10100602	0.10	0.21	0.10	0.21	0.00	0.00
10100604	0.00	0.00	0.00	0.00	0.00	0.00
10200601	23.14	2.79	23.14	3.20	0.00	0.42
10200602	3.53	4.10	3.53	4.10	0.00	0.00
10200603	1.24	2.39	1.24	2.39	0.00	0.00
10200604	0.08	0.21	0.08	0.21	0.00	0.00
10300601	0.94	0.31	0.94	0.44	0.00	0.12
10300602	1.73	1.58	1.73	1.58	0.00	0.00
10300603	1.24	1.46	1.24	1.46	0.00	0.00
20100201	16.78	21.81	16.78	30.53	0.00	8.72
20100202	2.07	1.31	2.07	1.31	0.00	0.00
20100205	0.00	0.00	0.00	0.00	0.00	0.00
20200201	2.42	4.09	2.42	5.72	0.00	1.63
20200202	14.61	10.56	14.61	10.56	0.00	0.00
20200203	2.17	5.38	2.17	5.38	0.00	0.00
20200204	0.44	0.35	0.44	0.35	0.00	0.00
20200205	0.00	0.00	0.00	0.00	0.00	0.00
20200252	0.07	0.33	0.07	0.33	0.00	0.00
20200253	0.83	0.84	0.83	0.84	0.00	0.00
20200254	0.06	0.32	0.06	0.32	0.00	0.00
20300201	4.88	1.35	4.88	1.89	0.00	0.54
20300202	0.55	1.55	0.55	1.55	0.00	0.00
20300203	4.13	5.76	4.13	5.76	0.00	0.00
20300204	0.21	0.16	0.21	0.16	0.00	0.00
39000602	0.07	0.13	0.07	0.18	0.00	0.05
39000603	0.09	0.22	0.09	0.22	0.00	0.00
39000699	1.20	4.33	1.20	4.33	0.00	0.00
Total	260.19	389.84	292.83	461.26	32.64	71.41

Table 15 CO and NO_x emissions from NG combustion by county for summer (tpd)

County	Summer Baseline		Case A		Case B		Case C		Case D	
	CO	NO _x	CO	NO _x	CO	NO _x	CO	NO _x	CO	NO _x
Alameda	5.46	4.17	5.50	4.46	5.67	4.46	5.46	4.18	5.46	4.17
Alpine	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Amador	0.33	1.32	0.33	1.75	0.36	1.76	0.33	1.32	0.33	1.32
Butte	0.38	0.55	0.41	0.68	0.52	0.68	0.38	0.55	0.38	0.55
Calaveras	0.02	0.02	0.02	0.03	0.02	0.03	0.02	0.02	0.02	0.02
Colusa	0.87	3.80	0.96	4.58	1.37	4.59	0.87	3.80	0.87	3.80
Contra Costa	9.77	8.50	9.81	9.74	10.00	9.75	9.77	8.71	9.77	8.50
Del Norte	0.04	0.02	0.04	0.03	0.06	0.03	0.04	0.02	0.04	0.02
El Dorado	0.13	0.09	0.13	0.09	0.16	0.10	0.13	0.09	0.13	0.09
Fresno	7.35	5.79	7.40	7.42	7.62	7.43	7.35	5.88	7.35	5.79
Glenn	0.23	1.14	0.23	1.19	0.24	1.19	0.23	1.14	0.23	1.14
Humboldt	0.97	4.42	0.98	5.33	1.06	5.33	0.97	4.90	0.97	4.42
Imperial	0.72	5.78	0.77	7.59	0.97	7.60	0.72	6.00	0.72	5.78
Inyo	0.03	0.02	0.03	0.02	0.04	0.02	0.03	0.02	0.03	0.02
Kern	16.52	41.78	17.09	53.09	19.63	53.31	16.52	44.71	16.52	41.78
Kings	1.39	2.60	1.39	3.53	1.39	3.53	1.39	2.60	1.39	2.60
Lake	0.06	0.04	0.07	0.05	0.12	0.05	0.06	0.04	0.06	0.04
Lassen	0.55	0.03	0.55	0.04	0.57	0.04	0.55	0.03	0.55	0.03
Los Angeles	66.83	29.28	67.08	34.45	68.26	34.49	66.83	30.74	66.83	29.28
Madera	0.32	0.80	0.34	0.89	0.42	0.89	0.32	0.80	0.32	0.80
Marin	0.40	0.31	0.41	0.39	0.44	0.39	0.40	0.31	0.40	0.31
Mariposa	0.01	0.01	0.02	0.01	0.02	0.01	0.01	0.01	0.01	0.01
Mendocino	0.22	0.20	0.23	0.25	0.26	0.25	0.22	0.20	0.22	0.20
Merced	1.43	1.56	1.46	2.01	1.57	2.02	1.43	1.56	1.43	1.56
Modoc	0.02	0.01	0.02	0.02	0.05	0.02	0.02	0.01	0.02	0.01
Mono	0.02	0.01	0.02	0.01	0.04	0.01	0.02	0.01	0.02	0.01
Monterey	5.10	7.79	5.15	10.70	5.40	10.71	5.10	8.45	5.10	7.79
Napa	0.41	0.34	0.41	0.38	0.45	0.38	0.41	0.34	0.41	0.34
Nevada	0.20	0.15	0.21	0.19	0.23	0.19	0.20	0.15	0.20	0.15
Orange	21.70	6.63	21.91	7.76	22.86	7.77	21.70	6.68	21.70	6.63
Placer	0.60	1.33	0.72	1.51	1.24	1.52	0.60	1.33	0.60	1.33
Plumas	7.88	0.55	7.88	0.76	7.90	0.76	7.88	0.55	7.88	0.55
Riverside	5.39	3.25	5.43	3.91	5.62	3.92	5.39	3.42	5.39	3.25
Sacramento	3.20	2.14	3.65	2.59	5.67	2.60	3.20	2.42	3.20	2.14
San Benito	0.13	0.59	0.14	0.79	0.15	0.79	0.13	0.59	0.13	0.59
San Bernardino	13.24	46.99	13.33	62.73	13.74	62.74	13.24	47.96	13.24	46.99
San Diego	47.60	11.29	51.22	14.04	67.32	14.05	47.60	12.44	67.32	13.64
San Francisco	3.80	1.97	3.83	2.24	3.94	2.25	3.80	2.06	3.80	1.97
San Joaquin	3.51	11.54	3.59	15.23	3.97	15.24	3.51	11.60	3.51	11.54
San Luis Obispo	1.88	0.94	1.92	1.10	2.07	1.11	1.88	0.97	1.88	0.94
San Mateo	2.54	1.32	2.56	1.49	2.65	1.49	2.54	1.32	2.54	1.32
Santa Barbara	3.58	4.82	3.60	5.91	3.69	5.92	3.58	4.83	3.58	4.82
Santa Clara	13.73	6.75	13.93	7.39	14.78	7.41	13.73	6.79	13.73	6.75
Santa Cruz	1.12	1.71	1.21	2.26	1.62	2.26	1.12	1.73	1.12	1.71
Shasta	1.37	2.45	1.50	3.00	2.07	3.01	1.37	2.47	1.37	2.45
Sierra	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Siskiyou	0.11	0.06	0.11	0.07	0.13	0.07	0.11	0.06	0.11	0.06
Solano	3.85	2.06	3.87	2.69	3.93	2.69	3.85	2.07	3.85	2.06
Sonoma	1.17	0.58	1.18	0.66	1.26	0.66	1.17	0.58	1.17	0.58
Stanislaus	1.82	6.22	1.86	8.37	2.06	8.38	1.82	6.27	1.82	6.22
Sutter	1.93	4.10	2.08	5.65	2.72	5.65	1.93	4.70	1.93	4.10
Tehama	1.17	0.86	1.18	0.98	1.21	0.98	1.17	0.86	1.17	0.86
Trinity	0.02	0.01	0.02	0.01	0.02	0.01	0.02	0.01	0.02	0.01
Tulare	1.59	1.45	1.62	1.85	1.75	1.85	1.59	1.45	1.59	1.45
Tuolumne	0.15	0.72	0.15	0.99	0.18	0.99	0.15	0.72	0.15	0.72
Ventura	6.77	3.04	6.92	3.80	7.63	3.81	6.77	3.29	6.77	3.04
Yolo	1.39	1.39	1.49	1.80	1.93	1.80	1.39	1.43	1.39	1.39
Yuba	0.12	0.22	0.14	0.26	0.21	0.26	0.12	0.22	0.12	0.22

Table 16 Increases in natural gas-related CO and NO_x emissions for summer (tpd)

County	Case A		Case B		Case C		Case D	
	CO	NO _x	CO	NO _x	CO	NO _x	CO	NO _x
Alameda	0.04	0.29	0.20	0.30	0.00	0.01	0.00	0.00
Alpine	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Amador	0.01	0.44	0.04	0.44	0.00	0.00	0.00	0.00
Butte	0.03	0.13	0.14	0.13	0.00	0.00	0.00	0.00
Calaveras	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00
Colusa	0.09	0.79	0.50	0.79	0.00	0.00	0.00	0.00
Contra Costa	0.04	1.24	0.23	1.25	0.00	0.21	0.00	0.00
Del Norte	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00
El Dorado	0.01	0.01	0.04	0.01	0.00	0.00	0.00	0.00
Fresno	0.05	1.63	0.27	1.65	0.00	0.09	0.00	0.00
Glenn	0.00	0.05	0.00	0.05	0.00	0.00	0.00	0.00
Humboldt	0.02	0.91	0.10	0.91	0.00	0.47	0.00	0.00
Imperial	0.04	1.82	0.24	1.82	0.00	0.23	0.00	0.00
Inyo	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00
Kern	0.57	11.31	3.11	11.52	0.00	2.93	0.00	0.00
Kings	0.00	0.94	0.00	0.94	0.00	0.00	0.00	0.00
Lake	0.01	0.01	0.06	0.01	0.00	0.00	0.00	0.00
Lassen	0.00	0.01	0.02	0.01	0.00	0.00	0.00	0.00
Los Angeles	0.25	5.17	1.43	5.21	0.00	1.46	0.00	0.00
Madera	0.02	0.09	0.10	0.09	0.00	0.00	0.00	0.00
Marin	0.01	0.08	0.05	0.08	0.00	0.00	0.00	0.00
Mariposa	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
Mendocino	0.01	0.04	0.04	0.04	0.00	0.00	0.00	0.00
Merced	0.03	0.45	0.14	0.46	0.00	0.00	0.00	0.00
Modoc	0.01	0.00	0.03	0.00	0.00	0.00	0.00	0.00
Mono	0.00	0.00	0.02	0.00	0.00	0.00	0.00	0.00
Monterey	0.06	2.90	0.31	2.91	0.00	0.65	0.00	0.00
Napa	0.01	0.04	0.04	0.04	0.00	0.00	0.00	0.00
Nevada	0.00	0.04	0.02	0.04	0.00	0.00	0.00	0.00
Orange	0.21	1.12	1.16	1.14	0.00	0.05	0.00	0.00
Placer	0.12	0.18	0.64	0.19	0.00	0.00	0.00	0.00
Plumas	0.00	0.21	0.02	0.21	0.00	0.00	0.00	0.00
Riverside	0.04	0.67	0.23	0.68	0.00	0.18	0.00	0.00
Sacramento	0.45	0.44	2.48	0.46	0.00	0.27	0.00	0.00
San Benito	0.00	0.20	0.02	0.20	0.00	0.00	0.00	0.00
San Bernardino	0.09	15.74	0.50	15.75	0.00	0.97	0.00	0.00
San Diego	3.62	2.75	19.73	2.76	0.00	1.15	19.73	2.35
San Francisco	0.03	0.27	0.14	0.28	0.00	0.08	0.00	0.00
San Joaquin	0.08	3.69	0.46	3.70	0.00	0.05	0.00	0.00
San Luis Obispo	0.03	0.16	0.19	0.17	0.00	0.03	0.00	0.00
San Mateo	0.02	0.17	0.11	0.17	0.00	0.00	0.00	0.00
Santa Barbara	0.02	1.10	0.12	1.10	0.00	0.01	0.00	0.00
Santa Clara	0.19	0.65	1.05	0.66	0.00	0.05	0.00	0.00
Santa Cruz	0.09	0.54	0.51	0.55	0.00	0.02	0.00	0.00
Shasta	0.13	0.55	0.69	0.56	0.00	0.01	0.00	0.00
Sierra	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Siskiyou	0.00	0.01	0.03	0.01	0.00	0.00	0.00	0.00
Solano	0.01	0.63	0.08	0.63	0.00	0.01	0.00	0.00
Sonoma	0.02	0.08	0.09	0.08	0.00	0.00	0.00	0.00
Stanislaus	0.04	2.15	0.25	2.16	0.00	0.04	0.00	0.00
Sutter	0.14	1.55	0.78	1.55	0.00	0.60	0.00	0.00
Tehama	0.01	0.12	0.04	0.12	0.00	0.00	0.00	0.00
Trinity	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Tulare	0.03	0.40	0.17	0.40	0.00	0.00	0.00	0.00
Tuolumne	0.01	0.28	0.04	0.28	0.00	0.00	0.00	0.00
Ventura	0.16	0.76	0.86	0.77	0.00	0.25	0.00	0.00
Yolo	0.10	0.41	0.54	0.41	0.00	0.04	0.00	0.00
Yuba	0.02	0.04	0.09	0.04	0.00	0.00	0.00	0.00

Table 17 CO and NO_x emissions from NG combustion by county in winter (tpd)

County	Winter Baseline		Case E		Difference Case E - Winter	
	CO	NO _x	CO	NO _x	CO	NO _x
Alameda	9.13	11.99	10.49	12.43	1.36	0.44
Alpine	0.01	0.01	0.01	0.01	0.00	0.00
Amador	0.37	1.50	0.39	1.96	0.02	0.46
Butte	0.78	1.65	0.95	1.84	0.17	0.19
Calaveras	0.03	0.04	0.03	0.05	0.00	0.01
Colusa	1.12	4.41	1.34	5.28	0.22	0.87
Contra Costa	12.45	14.22	13.47	15.58	1.02	1.35
Del Norte	0.05	0.03	0.06	0.04	0.01	0.01
El Dorado	0.18	0.23	0.20	0.25	0.03	0.02
Fresno	8.91	9.75	9.45	11.61	0.54	1.85
Glenn	0.27	1.23	0.28	1.29	0.01	0.06
Humboldt	1.25	5.33	1.37	6.30	0.12	0.97
Imperial	0.91	6.53	1.03	8.45	0.12	1.92
Inyo	0.03	0.03	0.04	0.03	0.01	0.01
Kern	19.12	62.78	20.82	77.28	1.69	14.50
Kings	1.44	2.70	1.44	3.64	0.01	0.94
Lake	0.08	0.07	0.11	0.09	0.03	0.01
Lassen	0.56	0.04	0.57	0.05	0.01	0.01
Los Angeles	82.57	66.26	86.69	72.32	4.13	6.06
Madera	0.45	1.32	0.52	1.47	0.07	0.15
Marin	1.24	2.08	1.55	2.20	0.31	0.11
Mariposa	0.02	0.01	0.02	0.02	0.00	0.00
Mendocino	0.31	0.46	0.36	0.52	0.04	0.06
Merced	1.79	2.59	1.94	3.12	0.15	0.53
Modoc	0.03	0.03	0.04	0.03	0.01	0.00
Mono	0.02	0.02	0.03	0.03	0.01	0.00
Monterey	5.92	10.18	6.28	13.24	0.36	3.07
Napa	0.73	1.02	0.86	1.07	0.13	0.05
Nevada	0.27	0.34	0.30	0.39	0.03	0.05
Orange	27.02	18.35	28.63	19.75	1.61	1.40
Placer	1.36	3.78	1.77	4.20	0.41	0.42
Plumas	7.89	0.56	7.90	0.77	0.01	0.21
Riverside	8.06	9.73	8.75	10.56	0.68	0.83
Sacramento	6.61	8.66	8.09	9.39	1.48	0.73
San Benito	0.21	0.80	0.24	1.01	0.03	0.21
San Bernardino	16.43	54.49	17.31	70.42	0.89	15.92
San Diego	55.79	16.40	64.68	19.34	8.89	2.94
San Francisco	6.14	6.95	7.01	7.32	0.87	0.37
San Joaquin	4.66	14.41	5.17	18.27	0.51	3.86
San Luis Obispo	2.37	2.55	2.55	2.84	0.18	0.28
San Mateo	4.61	5.70	5.37	5.96	0.76	0.26
Santa Barbara	4.45	6.96	4.68	8.15	0.23	1.19
Santa Clara	18.30	16.04	20.20	16.93	1.90	0.88
Santa Cruz	1.74	2.97	2.10	3.58	0.36	0.60
Shasta	1.89	3.28	2.25	3.90	0.37	0.62
Sierra	0.01	0.01	0.01	0.01	0.00	0.00
Siskiyou	0.12	0.07	0.13	0.09	0.01	0.02
Solano	4.79	4.04	5.13	4.70	0.33	0.67
Sonoma	2.26	2.95	2.67	3.09	0.41	0.13
Stanislaus	2.69	8.43	3.02	10.71	0.34	2.28
Sutter	2.42	4.63	2.80	6.23	0.38	1.60
Tehama	1.24	1.08	1.28	1.22	0.04	0.14
Trinity	0.02	0.01	0.02	0.01	0.00	0.00
Tulare	2.25	2.89	2.45	3.35	0.21	0.46
Tuolumne	0.16	0.74	0.18	1.02	0.02	0.28
Ventura	8.60	6.64	9.33	7.54	0.73	0.90
Yolo	1.92	2.33	2.25	2.79	0.33	0.46
Yuba	0.25	0.47	0.31	0.52	0.07	0.05

To evaluate the effect of changes in natural gas quality on vehicle emissions, two cases were simulated: the CNG Base Case and Case F. Both cases are based on the Summer Baseline. The CNG Base Case assumes a 5% market penetration of CNG vehicles for both the light-duty and heavy-duty markets, whereas the Summer Baseline has no explicit CNG vehicle category. There is little information about differences in emissions between CNG and conventional cars. In general, all vehicle emissions are regulated under the same standards, so there is no strong need under regulatory perspective to account for CNG vehicle emissions separately. Some information about the differences in emissions between conventional and CNG vehicles can be obtained from the assumptions by The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model by Argonne National Laboratory (<http://greet.es.anl.gov/>). This model is mainly used to evaluate lifecycle greenhouse gases emissions for fuels, but it includes emissions of criteria pollutants. The GREET model assumes that for CNG vehicles, tailpipe VOC emissions and VOC evaporative emissions are respectively 10% and 50% lower than the emissions from conventional vehicles. Tailpipe emissions of NO_x and CO are assumed the same for CNG and conventional vehicles.

Table 18 presents the emissions from on-road mobile sources for the Summer Baseline, the CNG Base Case, Case F, and the difference between Case F and the CNG Base Case. The only difference in emissions between Summer Baseline and CNG Base Case is the VOC emissions, which are 679 tpd in the CNG Base Case, 14 tpd less than in the Summer Baseline.

Case F simulates the changes in CNG vehicle emissions that result from of a natural gas quality change – an increase in WI by 50 BTU/scf – and the resulting air quality impacts. For Case F, CNG vehicles are assumed to make up 5% of all light-duty and heavy-duty vehicles. Assuming the emission sensitivity factors discussed in Section II.A.1, the resulting increase in statewide emissions from vehicles are 124 tpd, 23 tpd, and 45 tpd of CO, NO_x and VOC, respectively. The decrease in VOC emissions of 14 tpd produced by substituting 5% of conventional vehicles with CNG vehicles is more than offset by the 45 tpd increase produced by the increase in WI. The increase in NO_x emissions by 23 tpd, corresponds to a 0.7% increase with respect to the total statewide NO_x emissions of about 3500 tpd, and the estimated 45 tpd increase in VOC by 45 emissions corresponds to a 1.7% of the 2,600 tpd statewide emissions (ARB, 2009b).

Table 18 Emissions of CO, NO_x and VOC from mobile sources for Summer Baseline, CNG Base Case, and Case F by SCC (tpd).

Summer Baseline			
SCC	CO	NO _x	VOC
2201001000	2480	255	284
2201020000	2060	265	207
2201040000	635	97	55
2201070000	916	110	85
2230060000	5	13	1
2230070000	269	1024	62
Total	6365	1764	693

CNG Base Case			
SCC	CO	NO _x	VOC
2201001000	2480	255	278
2201020000	2060	265	203
2201040000	635	97	54
2201070000	916	110	84
2230060000	5	13	1
2230070000	269	1024	60
Total	6365	1764	679

Case F			
SCC	CO	NO _x	VOC
2201001000	2530	260	298
2201020000	2100	270	218
2201040000	648	99	57
2201070000	925	111	88
2230060000	5	13	1
2230070000	272	1034	62
Total	6480	1788	724

Case F – CNG Base Case			
SCC	CO	NO _x	VOC
2201001000	50	5	20
2201020000	40	5	15
2201040000	13	2	4
2201070000	9	1	4
2230060000	0	0	0
2230070000	3	10	2
Total	124	23	45

V Impacts of Gas Compositions on Air Quality

This section discusses air quality resulting from modeling the Summer Baseline and the Winter Baseline cases, and the air quality impacts resulting from the emissions increases in the six scenarios. Two meteorological episodes were simulated: July 7-13, 2005, a summer period with high observed ozone concentrations, and December 1-7, 2005, a winter period with high PM concentrations. Annual emissions were spatially and temporally disaggregated by SMOKE to approximate hourly emissions over the simulation domain. Figure 8 presents observed 8-hour average ozone concentrations and 24-hour average PM_{2.5} concentrations for 4x4 kilometers grid cells over California for Monday, July 13, the summer base case. Simulated 8-hour average ozone concentrations were high, with many areas in the Central Valley, San Jose, and Riverside, above 80 ppb (Figure 8a). Concentrations of PM_{2.5} on July 13 showed a spatial distribution typical for California, with peaks in the South Coast Air Basin and along the San Joaquin Valley (Figure 8b).

Figure 9 presents modeled hourly ozone concentrations together with observed ozone concentrations at five selected locations in California, and it shows that the model agrees well with observations. Overall, model performance is determined by the Mean Normalized Bias (MNB) and Mean Normalized Gross Error (MNGE), using Equations 8 and 9. Hourly observations are obtained from ARB's monitoring data recorded in 145 stations (ARB, 2012). Both MNB and MNGE are calculated using concentrations that are higher than 40 ppb, which is the background level for ozone. These metrics are recommended by the USEPA for model evaluation (U.S. EPA, 2007), and have been used extensively in the literature (Russell and Dennis, 2000; Eder and You, 2006; Appel et al., 2008; Foley et al., 2010).

$$\text{MNB} = \frac{1}{N} \sum_{i=1}^N \frac{C_M(x_i, t) - C_O(x_i, t)}{C_O(x_i, t)} \quad (9)$$

$$\text{MNGE} = \frac{1}{N} \sum_{i=1}^N \frac{|C_M(x_i, t) - C_O(x_i, t)|}{C_O(x_i, t)}, \quad (10)$$

where N is the number of observations in the region of interest during the campaign, $C_O(x_i, t)$ is the concentration of the i^{th} observation, and $C_M(x_i, t)$ is the corresponding modeled concentration at the same position and time. MNB and MNGE for July 13, 2005 are -7.6% and 29.3%, respectively. These values are within acceptable model performance parameters (U.S. EPA, 2007).

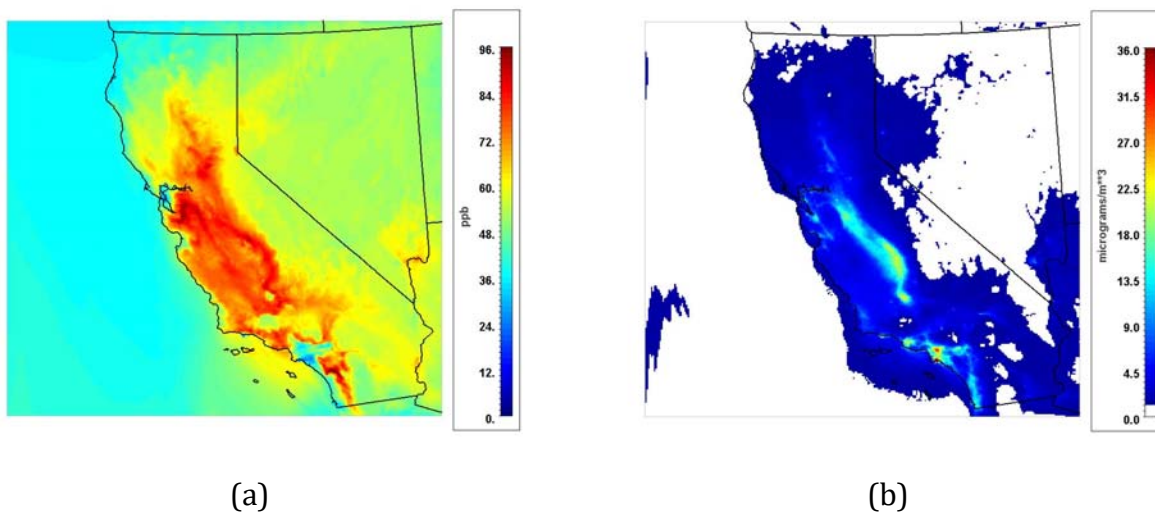


Figure 8 Ambient air concentrations for July 13, 2005: (a) 8-hour average ozone, (b) 24-hour average PM_{2.5}.

Figure 10 presents modeled and observed 24-hour average PM_{2.5} concentrations at all monitoring stations that reported data for July 13, 2005. Model MNB and MNGE, calculated with no cut-off value for 24-hour average concentrations of PM_{2.5}, are -2.8% and 31.9%, respectively.

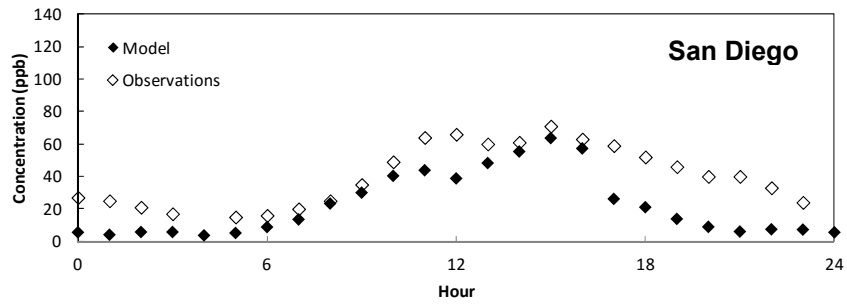
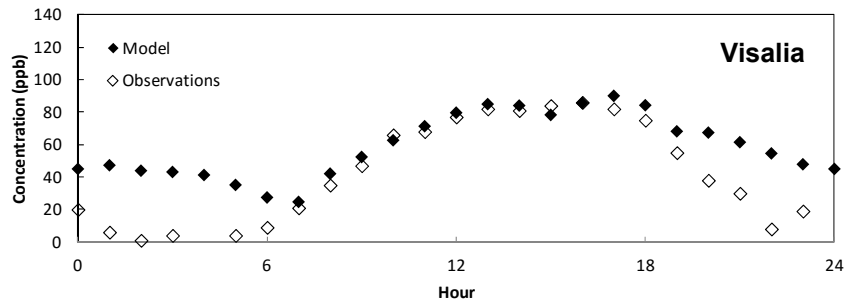
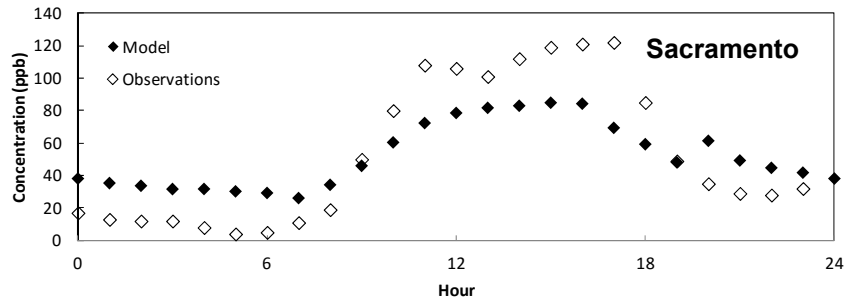
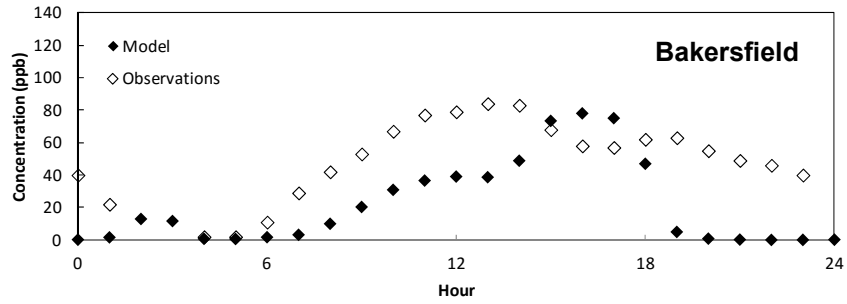
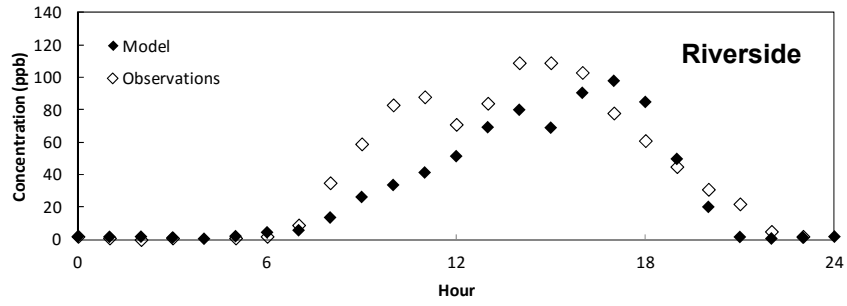


Figure 9 Modeled and observed hourly ozone concentrations for July 13, 2005 at selected locations

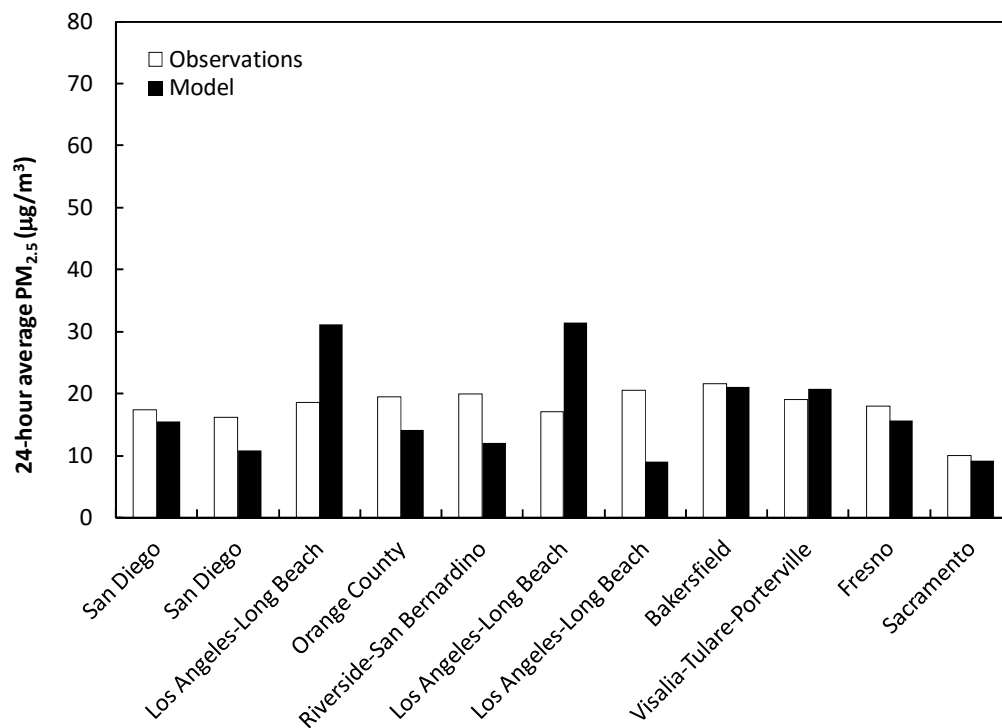


Figure 10 Modeled and observed 24-hour average PM_{2.5} concentrations for July 13, 2005 at selected locations

Figure 11 shows simulated 8-hour ozone concentrations and 24-hour PM_{2.5} concentrations for 4x4 km grid cells over California for Wednesday December 7, 2005, the Winter Baseline case. Simulated 8-hour ozone concentrations are low and below the state standard of 75ppb, which is typical for winter. The 24-hour average PM_{2.5} concentrations are higher for the Winter Baseline case than the Summer Baseline case, especially along the Sacramento and San Joaquin Valleys. Some regions in the Sacramento and San Joaquin Valleys experience 24-hour average PM_{2.5} concentrations higher than the 35 µg/m³ federal EPA standard.

Figure 12 presents winter modeled hourly ozone concentrations together with observed ozone concentrations for Wednesday December 7, 2005 at five selected locations in California, and it shows that the model also agrees well with observations. MNB and MNGE for December 7, 2005 are -10.9% and 12.0%, respectively. These values are within acceptable model performance parameters (U.S. EPA, 2007).

Figure 13 presents modeled and observed 24-hour average $PM_{2.5}$ concentrations at all monitoring stations that reported data for December 7, 2005. Model MNB and MNGE, calculated with no cut-off value for 24-hour average concentrations of $PM_{2.5}$, are -27.8% and 29.3%, respectively.

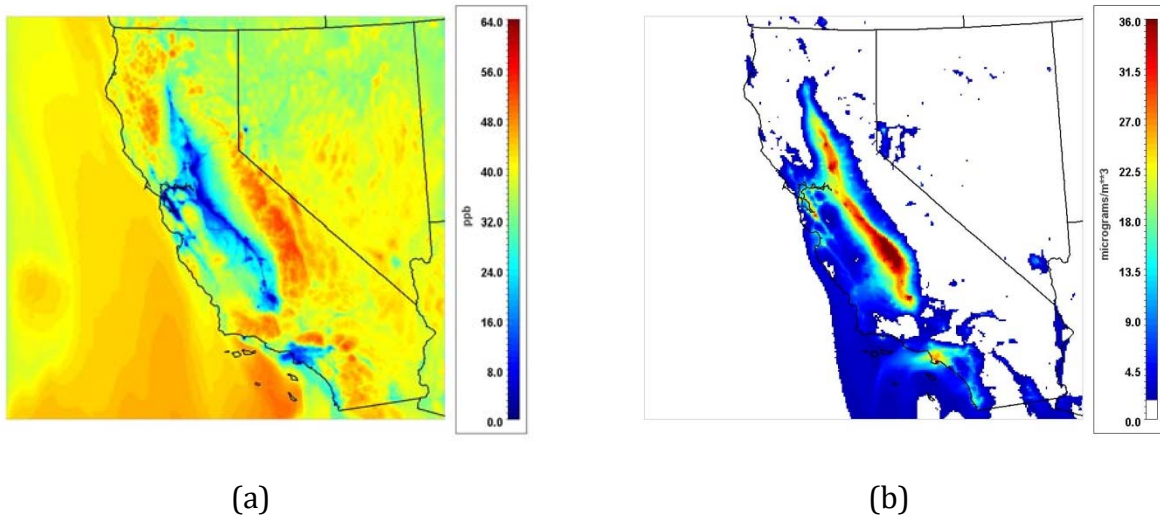


Figure 11 Modeled pollutant concentrations for December 7, 2005: (a) 8-hour average ozone, (b) 24-hour average $PM_{2.5}$.

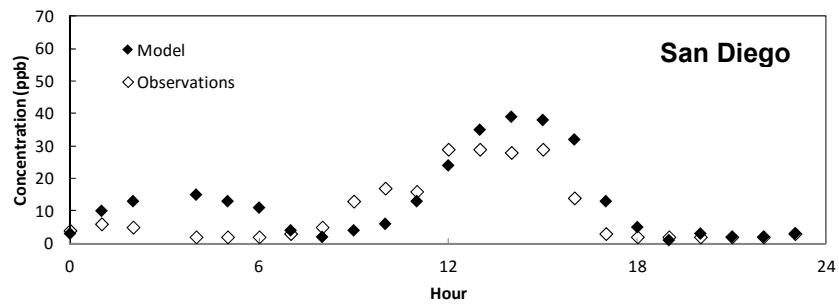
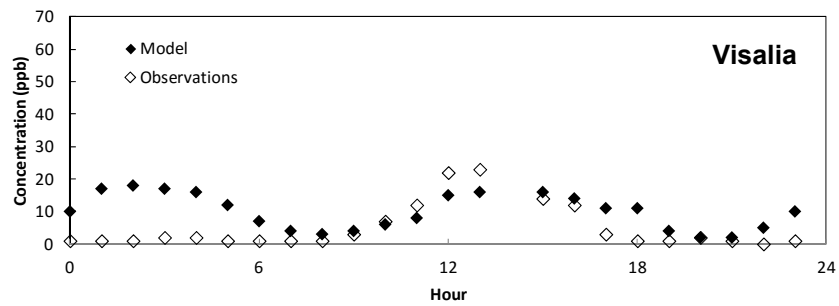
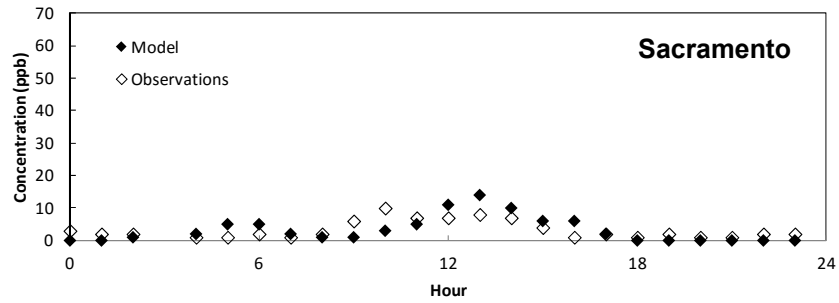
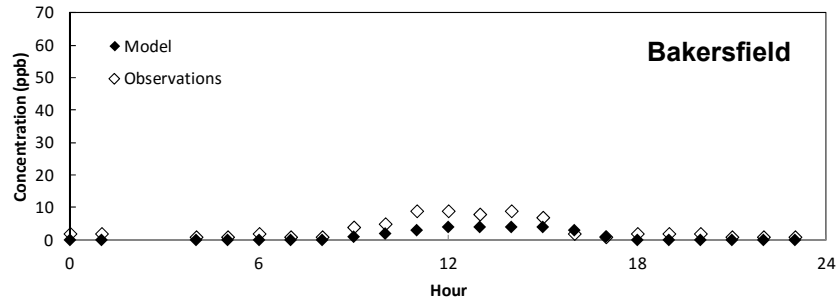
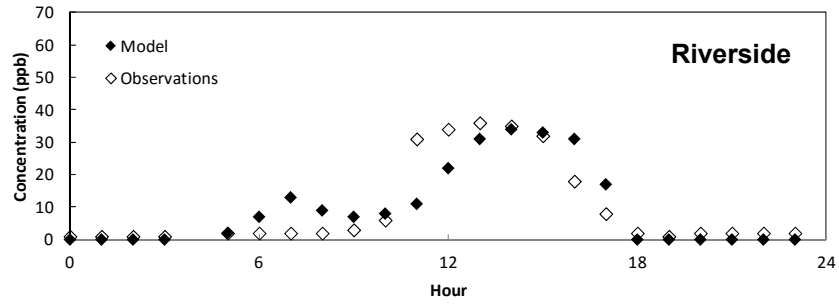


Figure 12 Modeled and observed hourly ozone concentrations for December 7, 2005 at selected locations

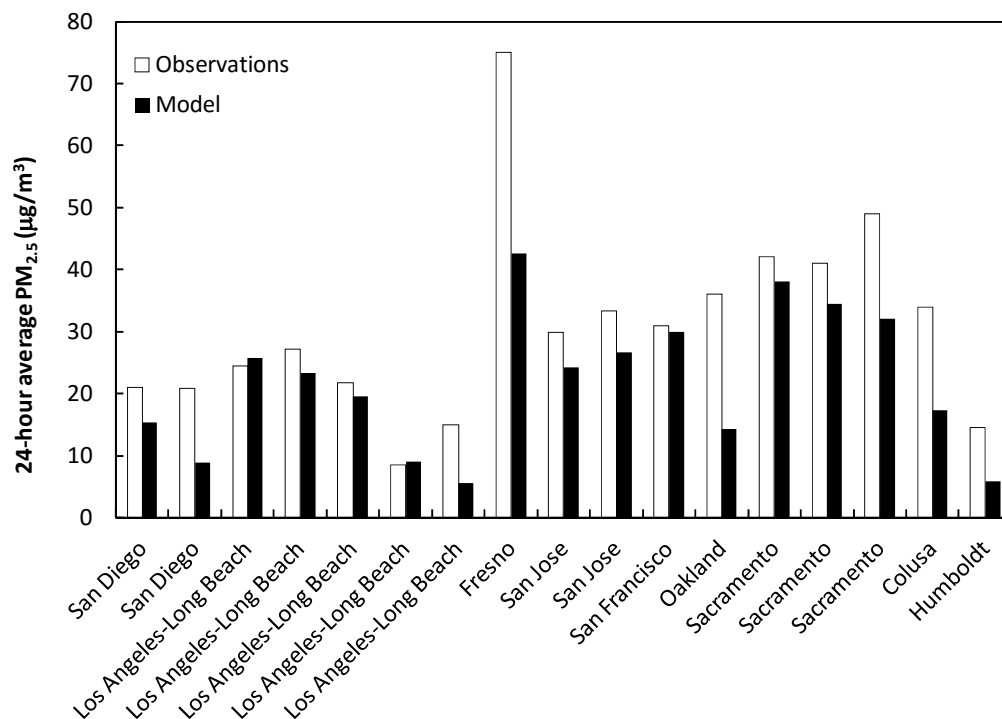


Figure 13 Modeled and observed 24-hour average PM_{2.5} concentrations for December 7, 2005 at selected locations

V.A Summary of Atmospheric Processes for Ozone and Particulate Matter

To enable understanding the presented simulation results, some of the processes that impact atmospheric ozone and particle concentrations are briefly discussed here.

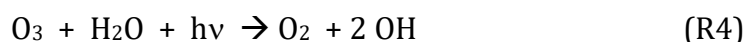
Ozone:

Ozone (O₃) is a secondary pollutant; it is not directly emitted, but rather is formed in the atmosphere through photochemical reactions of other pollutants. The formation of ozone is initiated by the photolysis of nitrogen dioxide (NO₂, a component of NO_x) in reaction R1:





Photolysis of NO₂ produces a single atom of oxygen (O) that reacts readily with molecular oxygen (O₂) present in the atmosphere, producing ozone by reaction R2. In the absence of other components, ozone is consumed by its reaction with NO to produce NO₂ and O₂ again by reaction R3, the ozone titration reaction. During the day, ozone also produces hydroxyl radical via photolysis and water addition by reaction R4:



VOC in the atmosphere can provide a catalyst to recycle NO back to NO₂ without undergoing ozone titration, hence contributing to the build-up of ozone. For example, an alkane VOC has a carbon-hydrogen bond (R-H) that can react with OH by reaction R5 to form H₂O and an alkyl radical R, which then reacts with NO to reform NO₂ by reaction R6.



Finally, ozone production can also be terminated by reaction R7, the combination of NO₂ with OH to form nitric acid (HNO₃), which can deposit to surfaces, effectively removing NO₂ from the atmosphere (Jacob, 1999).



Ozone formation is not a linear process. Ozone concentrations depend on NO_x concentrations, but also on a complex system of reactions that compete to increase (reactions R1, R2 and R6) and decrease (reactions R3 and R7) ozone. In Los Angeles, emissions of NO_x are high enough that consumption reactions prevail over production of ozone. Under these conditions, referred as a VOC-limited regime, an increase in VOC emissions tends to increase ozone concentrations, but increases in NO_x emissions can lead to a decrease in ozone (Jacob, 1999). This phenomenon has been regularly observed in the South Coast Air Basin during weekends, when emissions of NO_x are typically lower than on weekdays but measured ozone concentrations are statistically higher than during weekdays (Qin *et al.* 2004). In other areas where NO_x emissions are more moderate than in Los Angeles, such as the San Joaquin Valley, conditions for ozone build-up prevail, and an increase in NO_x emissions generally produces an increase in ozone concentration.

Particulate Matter:

Unlike ozone, particulate matter (PM) is both emitted and formed in the atmosphere. Main sources of particulate matter emissions include combustion, suspension of material from

natural processes and human activity, and from wear and tear of tires and brakes. Fine particles may be formed by the reaction of nitric and sulfuric acid with ammonia to form ammonium nitrates and ammonium sulfates. Because ammonia emissions from cattle and agricultural operations can be high, formation of ammonium nitrate and sulfates is an important PM source in the Central Valley and in Riverside and San Bernardino Counties where those activities are common. In general, increasing NO_x emissions leads to greater formation of atmospheric nitric acid and hence, an increase in secondary PM formation.

V.B Discussion of Scenarios

For each of the six simulated scenarios, incremental changes in 8-hour average ozone and 24-hour average PM_{2.5} concentrations are presented in Figure 14 and Figure 15, respectively. All scenarios assume an increase in NO_x emissions with respect to their reference case. Cases A through D have the Summer Baseline case as reference. Case E has the Winter Baseline as reference, and Case F has the CNG Base Case as reference.

Cases A and B simulate the effects of increasing WI by 50 BTU/scf on all stationary NG combustion sources with the only difference being the emission sensitivity factor for residential appliances. These two cases present the highest simulated increases in emissions in the summer, with nearly 2% increase in NO_x emissions with respect to the baseline. As discussed above, a moderate increase in NO_x emissions in an area with high baseline emissions, such as Los Angeles, can slightly reduce ozone concentration. In contrast, NO_x emission increases in other areas of the state – such as the San Joaquin and Sacramento Valleys – lead to increases in 8-hour ozone concentrations of approximately 1 ppb.

Case C focused on changing emissions only from the electric utility sector, resulting in 0.3% increase in statewide NO_x emissions with respect to the Summer Baseline, a smaller increase compared to Cases A and B. As a result, the impacts of large electricity generation point sources on ozone concentrations observed in Case C are small, less than 0.2 ppb in all cases.

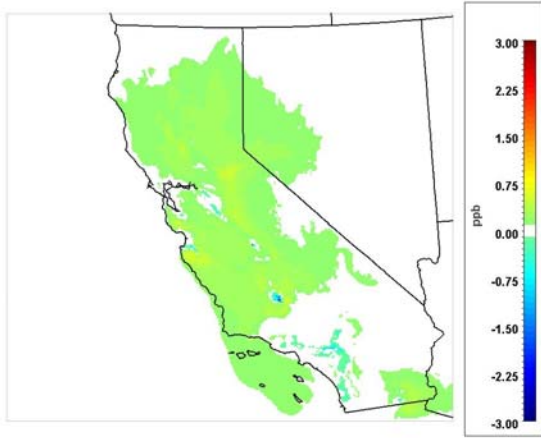
Case D simulate the effects of increasing WI by 50 BTU/scf on all stationary NG combustion sources in San Diego County only. Emissions in the other counties are not affected by the scenario, so any effects on air quality outside San Diego County is due to transport of pollutants. For the conditions of Case D, emissions originating in San Diego County increase ozone concentrations in San Diego County by up to 0.2 ppb, and but the effect on ozone concentrations in Los Angeles are negligible. These results illustrate that emissions from San Diego can be transported northwards within days (these simulations represent a

week) and reach areas in the South Coast air Basin. Nonetheless, the impacts on ozone in Los Angeles are also less than 0.2 ppb.

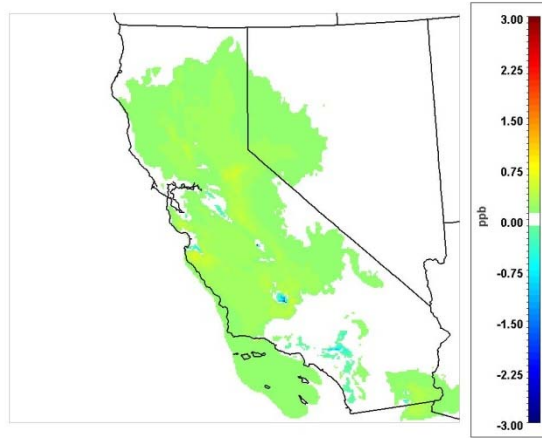
Case E assumes the emission sensitivity factors that Case B for a winter episode, and hence it evaluates the winter time air quality impacts of a 50 BTU/scf WI increase while assuming Maximum Burner Sensitivity values for the emission sensitivities of burners and equipment. In Case E, statewide NO_x emissions increase by 2% with respect to the Winter Baseline. With lower solar radiation and lower temperatures in winter, ozone formation is limited compared to Case B in the summer. At this level of increased NO_x emissions, ozone titration prevails in many regions of the state, leading to reduced 8-hour average ozone concentrations as seen in Figure 12.

Case F is intended to evaluate the air quality impacts of changing emissions from CNG vehicles, and it is the only case that assumes an increase in VOC emissions in addition to an increase in NO_x emissions. NO_x emissions from CNG vehicles increase statewide NO_x emissions by 0.7%, which is smaller than the 1.8% increase seen in Case B, which evaluated emission changes from only stationary sources. Statewide VOC emissions for Case F increase by 1.7% with respect to CNG Base Case, causing ozone concentrations in Los Angeles to increase by nearly 1 ppb, in contrast to Case B, where 8-hour average ozone concentrations decreased by nearly 1 ppb due to a larger NO_x emission increase.

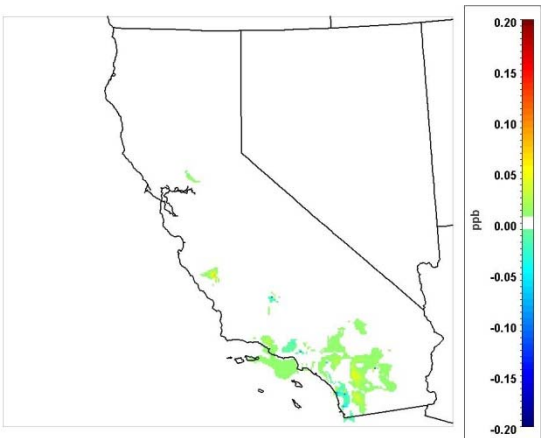
Changes in direct emissions of PM_{2.5} were not considered in any of the simulation scenarios, so the changes in 24-hour PM_{2.5} concentrations presented in Figure 13 are solely due to secondary formation of particles in the atmosphere. Nitric acid can be formed in the atmosphere by the oxidation of emitted NO_x. Fine particles form from the reaction of gas-phase nitric acid and ammonia. As for ozone, the cases with the greatest changes in PM_{2.5} concentrations are Cases A, B and C, because these cases have the greatest increases in NO_x emissions. The largest increases in PM_{2.5} concentrations occur along the San Joaquin Valley, where the increased NO_x emissions from combustion of higher WI natural gas form nitric acid, which then reacts with ammonia emitted from farming and cattle operations to create ammonium nitrate PM. In general, the impacts of changing natural gas combustion emissions on PM_{2.5} concentrations throughout the state is small, and the changes in 24-hour average concentrations are lower than 0.3 µg/m³ for all modeling cases.



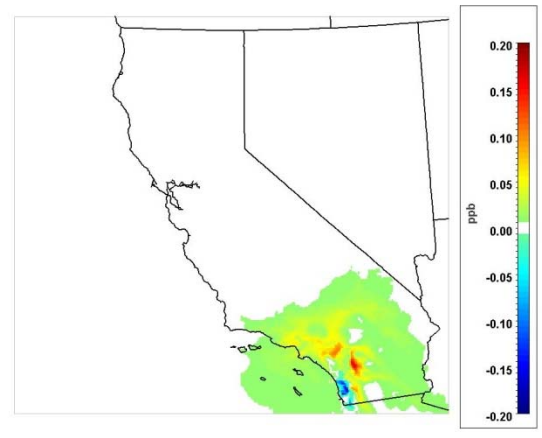
Case A – Summer Baseline



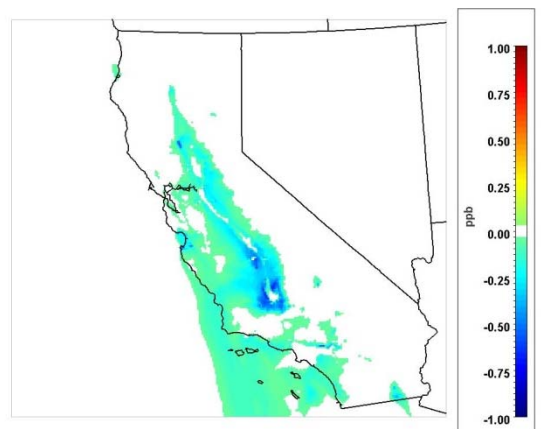
Case B – Summer Baseline



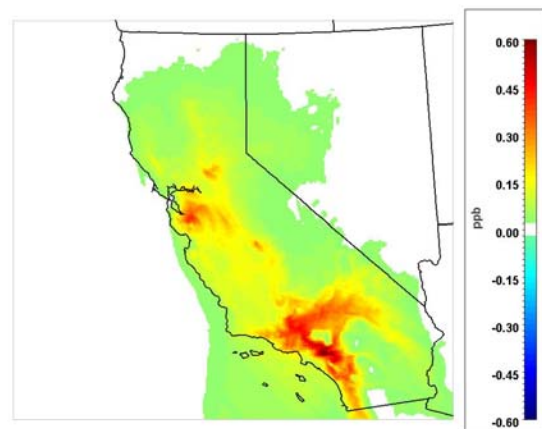
Case C – Summer Baseline



Case D – Summer Baseline

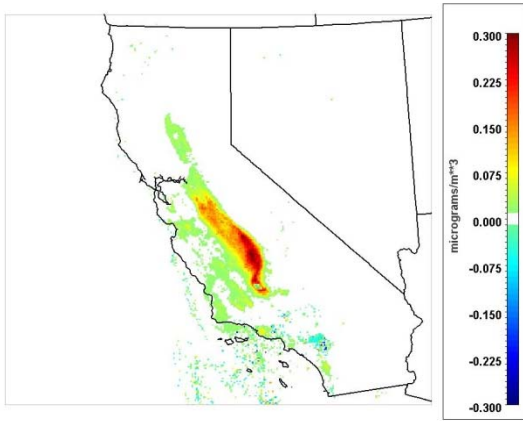


Case E – Winter Baseline

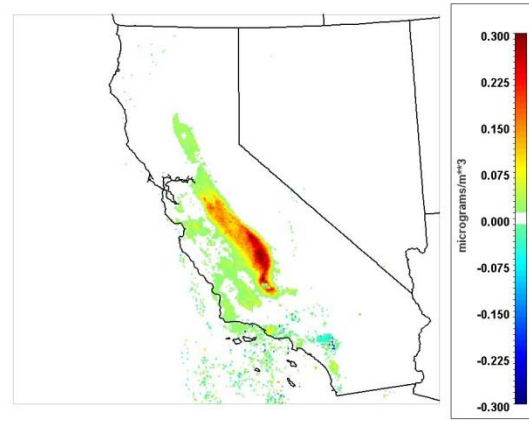


Case F – CNG Base Case

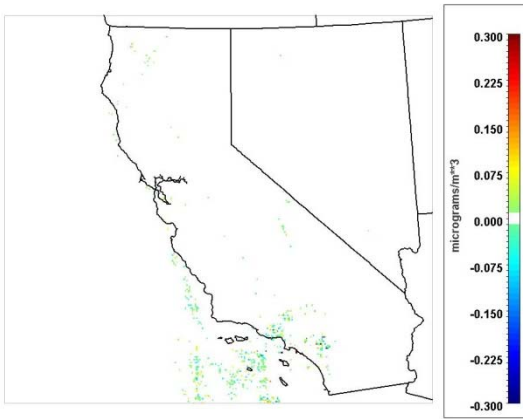
Figure 14 Incremental changes in 8-hour average ozone concentrations for the six modeling cases.



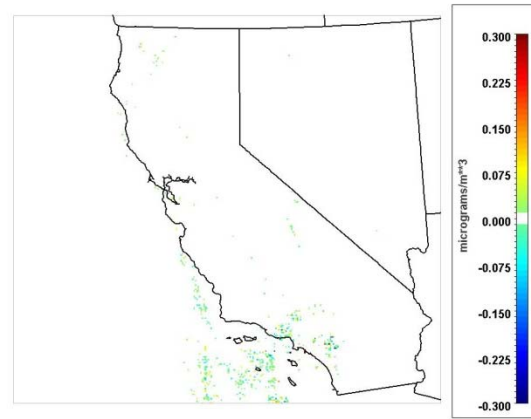
Case A – Summer Baseline



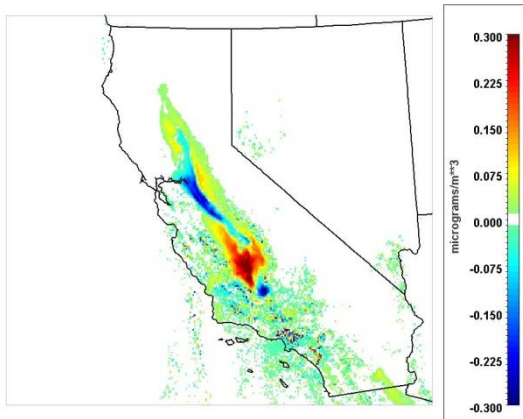
Case B – Summer Baseline



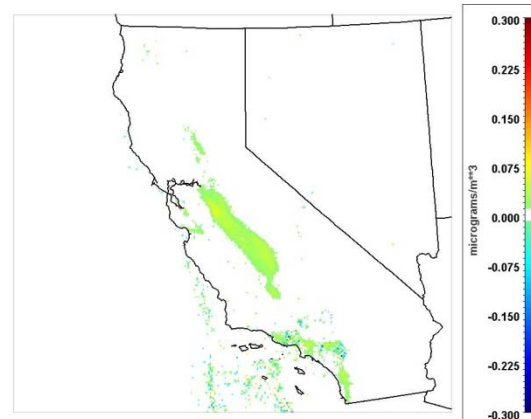
Case C – Summer Baseline



Case D – Summer Baseline



Case E – Winter Baseline



Case F – CNG Base Case

Figure 15 Incremental changes in 24-hour average $PM_{2.5}$ concentrations for the six modeling cases.

VI Summary and Future Work

This report demonstrates the use of the TEMPLES model to determine potential impacts of changing natural gas composition on air pollutant emissions and air quality. Six scenarios involving combustion emissions from residential, commercial, industrial, and transportation sectors were simulated. The results show industrial and commercial sectors are the main contributor to ozone changes. These changes are due to the high sensitivity of ultra-low NO_x burners with respect to changes in WI, based on experimental data (SoCalGas, 2004, 2006a, and 2006b). However, the data are scarce and are dated, nearly a decade old. More experimental data for small industrial burners, internal combustion engines and turbines are needed to improve the simulation results and to reduce the uncertainties. The present simulations used the 2005 U.S. EPA National Emissions Inventory as the baseline. This baseline would be replaced with ARB's 2012 emission inventory when it becomes available. In addition, detailed fugitive emissions from natural gas production, processing, transmission and distribution will be included in future work.

VII References

Appel K. W., Bhawe P. V., Gilliland A. B., Sarwar G., Roselle S. J., 2008. Evaluation of the community multiscale air quality (CMAQ) model version 4.5: Sensitivities impacting model performance; Part II - particulate matter. *Atmospheric Environment*, 42, 6057-6066.

California Air Resources Board, 2009a. CEPAM: 2009 Almanac - Population and Vehicle Trends Tool. Available at:
http://www.arb.ca.gov/app/emsinv/trends/ems_trends.php
(Accessed: December, 2013).

California Air Resources Board, 2009b. CEPAM: 2009 Almanac - Standard Emissions Tool. Available at: <http://www.arb.ca.gov/app/emsinv/fcemssumcat2009.php>
(Accessed: December, 2013).

California Air Resources Board, 2012. Database: California Air Quality Data - Selected Data Available for Download. Available at: <http://www.arb.ca.gov/aqd/aqdcdd/aqdcddld.htm>
(Accessed: December, 2013).

Baez A., 2010. Boiler and Process Heater Profile by Size in the South Coast Air Basin of California. South Coast Air Quality Management District, Internal Communication.

Crawford R., and Lyons J., 2009. Effects of Gas Composition on Emissions from a Light-Duty Natural Gas Vehicle. Prepared for Southern California Gas Company, *Sierra Research Report No. SR2009-11-01*.

Crawford R., and Lyons J., 2010. Effects of Gas Composition on Emissions from a Heavy-Duty Natural Gas Engines. Prepared for Southern California Gas Company, *Sierra Research Report No. SR2010-02-01*.

Crawford R., Lyons J., Heiken J., 2009. Effects of Gas Composition on Emissions of Heavy-Duty Natural Gas Engines. *Sierra Research Report No. SR2009-10-1*.

Eder B., Yu S., 2006. A performance evaluation of the 2004 release of Models-3 CMAQ, *Atmospheric Environment*, 40, 4811-4824.

Foley K. M., Roselle S. J., Appel K. W., Bhawe P. V., Pleim J. E., Otte T. L., Mathur R., Sarwar G., Young J. O., Gilliam R. C., Nolte C. G., Kelly J. T., Gilliland A. B., Bash J. O., 2010. Incremental testing of the Community Multiscale Air Quality (CMAQ) modeling system version 4.7. *Geoscientific Model Development*, 3, 205-226.

Gas Technology Institute, 2006. Light-Duty CNG Vehicle Fuel Composition Study. Topical Report, *GTI Report #20245*.

Gas Technology Institute, 2006. Natural Gas Variability in California: Environmental Impacts and Device Performance-Literature Review and Industrial Burner Evaluations. California Energy Commission, Contract Number: CEC-500-2006-096.

General Electric, 2005. Presentation to SoCalGas: Fuel Flexibility in GE LM Engines.

Available at:

http://www.socalgas.com/documents/business/gasquality/elec_gen_fuel_flexibility_ge_lm_engines.pdf

(Accessed: December, 2013.)

Harte E., 2009. 2008 Southern California Heavy-Duty CNG Vehicle Report, Southern California Gas Company and San Diego Gas & Electric. Available at:

http://www.socalgas.com/documents/business/gasquality/SoCalGasSDG&E_2008SouthernCaliforniaHDCNGVehicleReport.pdf

(Accessed: December, 2013.)

Jacob D.J., 1999. Introduction to Atmospheric Chemistry. Princeton University Press, USA.

KEMA, 2010. 2009 California Residential Appliance Saturation study, prepared by KEMA Inc. for the California Energy Commission, Contract Number: CEC-200-2010-004-ES

Klug V.L., Lobscheid A.B., Singer B.C., 2011. Cooking Appliance Use in California Homes – Data Collected from a Web-Based Survey. Indoor Environment Department, Environmental Energy Technologies Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Martinez A.S., Jani A., and Dabdub D., 2014. Emission Factor Estimation in Regional Air Quality Studies of Residential Natural Gas Fuel Interchangeability. *Fuel*, 119, 129-140.

NCEP, 2005. National Centers for Environmental Prediction/National Weather Service/NOAA/U.S. Department of Commerce. 2000, updated daily. NCEP FNL Operational Model Global Tropospheric Analyses, continuing from July 1999. Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory. <http://rda.ucar.edu/datasets/ds083.2>. (Accessed: January, 2012)

Qin Y., Tonnesen G.S., Wang, Z., 2004. Weekend/weekday differences of ozone, NO_x, CO, VOCs, PM₁₀ and the light scatter during ozone season in southern California. *Atmospheric Environment*, 38, 3069–3087.

Russell A., Dennis R., 2000. NARSTO critical review of photochemical models and modeling. *Atmospheric Environment*, 34, 2283-2324.

Singer B.C., Apte M.G., Black D.R., Hotchi T., Lucs D., Lunden M.M., Mirer A.G., Spears M., Sullivan D.P., 2009. Natural Gas Variability in California: Environmental Impacts and Device Performance – Experimental Evaluation of Pollutant Emissions from Residential Appliances. Lawrence Berkeley National Laboratory, *Report Number: LBNL 2897-E*.

Southern California Gas Company (SoCalGas), 2004. Gas Quality and LNG Research Study. Appendix B-4: Ultra-Low NO_x Steam Boiler. Available at:
<http://www.socalgas.com/documents/business/gasquality/B4UltraLowNOxSteamBoilerReport.pdf>
(Accessed: December, 2013.)

Southern California Gas Company (SoCalGas), 2006a. Equipment Studies, 2005-2006 SoCalGas Equipment Tests. Low NO_x Boilers-Expanded Testing, Low NO_x Steam Boiler. Available at:
<http://www.socalgas.com/documents/business/gasquality/LowNOxSteamBoiler.pdf>
(Accessed: December, 2013.)

Southern California Gas Company (SoCalGas), 2006b. Equipment Studies, 2005-2006 SoCalGas Equipment Tests. Low NO_x Boilers-Expanded Testing, Steam Boiler. Available at:
<http://www.socalgas.com/documents/business/gasquality/steamboilerpremixedguntype.pdf>
(Accessed: December, 2013.)

Timmons S., 2009. Natural Gas Fuel Effects on Vehicle Exhaust Emissions and Fuel Economy. *Final Report for Southwest Research Institute (SwRI) Project No. 03-13721.01.200*.

Tickel T., Aronchil G., Wagner, J., 2009. Natural gas in California: Environmental Impacts and Device Performance - Industrial Burner Evaluations: Radiant Tube Burner Interchangeability Test Report. Gas Technology Institute for the California Energy Commission, Contract Number: CEC-500-05-026.

Tickel T., Wagner J., 2009. Natural Gas in California: Environmental Impacts and Device Performance - Industrial Burner Evaluations: Infrared Burner Interchangeability Test Report. Gas Technology Institute for the California Energy Commission, Contract Number: CEC-500-05-026.

U.S. EPA, 2007. Guidance on the Use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM_{2.5}, and Regional Haze Office of Air Quality Planning and Standards, Air Quality Analysis Division, Air Quality Modeling Group, United States Environmental Protection Agency, EPA-454/B-07-002, April 2007. Research Triangle Park, North Carolina, USA

U.S. EPA, 2011. Technology Transfer Network Clearinghouse for Inventories & Emissions Factors. 2005 National Emissions Inventory. Available at:
<http://www.epa.gov/ttn/chief/emch/index.html>
(Accessed: December, 2013.)

Appendix A

USER'S GUIDE FOR TEMPLES/CMAQ

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User's Guide for TEMPLES/CMAQ

VIII Introduction

This document is a User's Guide to accompany the TEMPLES (Tool for Emissions Processing of LNG Expansion Scenarios)/CMAQ (Community Multiscale Air Quality model) software package (in parts suggested, in others developed) for the California Air Resources Board (ARB) by the Computational and Environmental Sciences Laboratory (CES) at the University of California, Irvine. The guide provides both an overview of the necessary input files and run sequence to utilize TEMPLES/CMAQ as well as a simple example that the user can recreate. By following the example outlined in this guide and reviewing the background material provided in progress reports from the development of the TEMPLES/CMAQ software, the user will become familiar with all the basic functions necessary to begin developing scenarios and hypotheses to test the effects of changing natural gas composition on air quality in California. Additionally, this guide provides an introduction to commonly-used methods of visualizing simulation results using the VERDI (Visualization Environment for Rich Data Interpretation) software package. Finally, this guide reinforces the material covered at the 2-day TEMPLES/CMAQ workshop presented for ARB by CES on January 24-25, 2013.

TEMPLES/CMAQ is a simulation platform for studying the air quality impacts of changes in natural gas composition within California. Originally, the application of the software envisioned scenarios of Liquefied Natural Gas (LNG) expansion within the state, but it is written generally for investigation of multiple sources of natural gas. The software is built from a suite of modeling packages that include open-access and community-developed codes as well as new modules developed specifically for this task by CES at UCI. The goal is to provide a package that only requires the user to specify information related to the natural gas source and the effects of composition changes on emissions from natural gas equipment. All other information required for simulating air quality (geography, meteorology, atmospheric chemistry, etc...) has been built into the platform so that it is transparent to the user. The user can simply select a representative case for these aspects (such as a warm summer day or a cool winter day) and be able to obtain information on the resultant changes in air quality under any user-defined natural gas supply scenario.

IX Hardware and Software Requirements

TEMPLES/CMAQ is a powerful simulation platform intended for operation on UNIX-based computers with substantial computing power. It is designed to take full advantage of the capabilities provided by the computing hardware and operating system, including parallel processing. However, to become familiar with VERDI/CMAQ or to test smaller-scale simulation scenarios, a more modest hardware configuration may be used. A more modest configuration will

not result in a loss of accuracy or capability of the model, but in significantly longer simulation times. The most basic required configuration is as follows:

Minimum Hardware Requirements

- UNIX operating system
- Single 1 GHz processor
- 1 GB RAM
- 1 TB hard disk storage (for run-time storage and long-term archiving of results)

On a system with the above configuration, simulating one week of statewide emissions and air quality with the default grid resolution of 4 km by 4 km and a solution time step of 1 hour would require approximately one full month of wall clock time to execute. Additionally, this configuration does not take full advantage of the software's capabilities as it necessarily processes the simulation in serial mode rather than in parallel. A recommended minimum practical configuration would therefore be as follows:

Minimum Practical Hardware Configuration

- Ubuntu Linux operating system
- 8 dual-core 2.5 GHz processors
- Network cabling and switch for processors to communicate (if on individual PCs)
- 2 GB RAM per processor
- 80 GB internal storage (for run-time storage)
- 10 TB IDE-SCSI RAID 5 Array (for long-term, secure archiving of results)

This configuration takes advantage of more of the capabilities for which TEMPLES/CMAQ was designed and allows for the same one-week simulation to be completed in significantly less time, about 2 days of wall clock time. A preferred configuration may reduce the simulation time further by a factor of 2-4, potentially at a cost only slightly higher than the minimum practical configuration. The preferred configuration also has the advantage that all processors are integrated in a single unit and were designed to communicate with one another. Therefore, additional network communications switches and cables do not need to be purchased for the following preferred configuration:

Preferred Hardware Configuration

- 64-core blade built on AMD Opteron 6274 hardware, at 2.2Ghz per processor

- 256 GB DDR3 RAM at 1600 MHz
- 1TB internal storage (for run-time storage)
- 10 TB IDE-SCSI RAID 5 Array (for long-term, secure archiving of results)

Additionally, basic mouse, keyboard, and monitor hardware will be required; speakers are not necessary.

IX.A Required Components of TEMPLES/CMAQ

In typical usage, users only need to interact with the two major components of the software, namely the TEMPLES and CMAQ modules. TEMPLES is a pre-processor for emissions-related input files of the simulation; CMAQ is the simulation framework and calculation module. However, CMAQ relies on the integration of several other modules, which are themselves stand-alone software packages, to provide all of the necessary input data to properly specify a simulation scenario. These include WRF (Weather Research and Forecasting model) for meteorology, SMOKE (Sparse Matrix Operator Kernel Emissions) for emissions allocation (TEMPLES interacts with SMOKE), CB05 (Carbon Bond 2005) for specification of chemistry in the atmosphere, and MM5/TERRAIN to specify the geographical features of the simulation domain.

The TEMPLES/CMAQ tool was developed assuming that typical usage would not require access to and interaction with all of these modules. Based on the proposed goals of the software's usage, only emissions-related data would be modified for the majority of the potential simulations. Maintaining consistent data for the other aspects of simulation (geography, meteorology, and chemistry) allows for clearer interpretation and comparisons between simulated scenarios. Thus, WRF, CB05, and MM5/TERRAIN are not explicitly required on the simulation computer. Instead, the software package contains files of data generated by previously operating each of these modules. These can then serve as consistent input files to TEMPLES/CMAQ for geography, meteorology, and chemistry. In particular, WRF has been operated to simulate seasonally-specific weather events. To develop customized input files (for example a new weather event not previously simulated), the appropriate module would need to be installed and operated on the simulation computer. Care is needed to review all the related documentation of that module and ensure that execution is properly carried out. It is recommended to use the most current version of the module as of January 2013, but not any version newer than that to avoid compatibility issues.

TEMPLES, CMAQ, and SMOKE all need to be installed on the simulation computer to use the TEMPLES/CMAQ tool. TEMPLES does not require any additional software modules to support its operation. However, SMOKE and CMAQ use specific software packages for data storage and input and output message passing: netCDF, MPICH, and IOAPI. It is suggested that CMAQ v4.7.1 is installed for use with this software package. Both SMOKE and CMAQ can be downloaded from CMAS (Community Modeling and Analysis System) at <http://www.cmascenter.org/>. Special care must be taken to ensure that a consistent FORTRAN compiler (Gfortran from the GCC (GNU Compiler Collection), ifort from Intel, or pgif from PGI) is used in building SMOKE, CMAQ, netCDF,

and IOAPI. Gfortran is the recommended compiler; if that does not work with the hardware architecture then try either ifort or pgif. Further information and guidance for installing CMAQ can be found at

http://www.cmascenter.org/help/model_docs/cmaq/4.7.1/CMAQ_4.7.1_OGD_28june10.pdf.

IX.B Additional Software to Interact with TEMPLES/CMAQ

Modification of the TEMPLES input files can be accomplished with any simple or feature-rich text editor. The editing may be completed either on the UNIX-based simulation computer or another computer, as long as the file is properly transferred to the simulation computer. In the UNIX environment, Pico provides a simple editing environment. Emacs offers a graphical and more feature-rich interface. Additionally, Emacs is purpose-built with special features and shortcuts for editing FORTRAN files and is the preferred option for both new users and advanced users who modify the modeling software for purposes beyond its original scope. Both text editors are easily found online and installed on the simulation computer. Emacs can also be used in a Windows environment as an alternative to Microsoft Word, Excel and Notepad, any of which could also be used. Finally, the visualization software VERDI is recommended for post-simulation processing. This package is also freely available from the CMAS website.

X Installation Guide

Each component mentioned above should be installed according to the documentation found on its website. The following order of installation steps is recommended when setting up the simulation computer.

X.A Order of Installation

1. Ubuntu/Linux operating system
2. Text editor (Pico is typically included with the operating system; Emacs must be installed separately)
3. If desired, a text editor or spreadsheet program
4. FORTRAN compiler
5. MPICH

6. netCDF and IOAPI (Remember to take note of the FORTRAN compiler utilized in this step and reference the CMAQ Installation documentation to ensure that environmental variables are set properly for this and the following step)
7. CMAQ
8. SMOKE
9. TEMPLES
10. VERDI (May be on the simulation computer or on another computer)

X.B Installing TEMPLES

TEMPLES does not require special installation. Rather, TEMPLES is a collection of pre-operated input data, input files related to the definition of natural gas supply scenarios, and a shell script that automates the execution of UNIX command-line operations. Thus, it is only required that the files are located in the proper directories. The supply scenario input files are:

- PARAMETERS.H
- MEASUREMENTS.DAT
- WOBBEINDEX.DAT
- XREF_TABLE.DAT
- SETPROGRAM

and the shell script is EMPROC.SH.

The exact location of the folder containing these files is not important; however, they must all be in the same folder. Thus, the folder may be placed directly within the user's home directory or within a subdirectory that is convenient for collecting, archiving, and maintaining simulation files.

XI Understanding Input Text Files for TEMPLES/CMAQ

The header file PARAMETERS.H and the three text files listed above, MEASUREMENTS.DAT, WOBBEINDEX.DAT, and XREF_TABLE.DAT are the main input files through which the user defines natural gas scenarios for TEMPLES/CMAQ. In brief, the header file PARAMETERS.H initializes the data vector and matrix sizes for the .DAT files and TEMPLES. Each .DAT file represents a different aspect of the scenario definition. The file WOBBEINDEX.DAT provides the statewide spatially-resolved data of natural gas composition changes for a particular scenario. These gas compositions are indicated by differences in the average Wobbe Index (WI) and Lower Heating Value (LHV)

relative to a baseline case. MEASUREMENTS.DAT and XREF_TABLE.DAT are related to the impact scenario. The impact scenario is defined as the combination of the simulation's state-wide populations of natural gas-burning technologies and the technology-specific changes in emissions as a function of natural gas composition. MEASUREMENTS.DAT contains the technology-specific pollutant emission changes resulting from changes in natural gas composition. XREF_TABLE.DAT matches the technology types in MEASUREMENTS.DAT to broader categories used in SMOKE. Therefore this input file determines the proportional contribution of each technology to these broader technology classification groups.

These input files may all be modified in a text editor on the simulation computer or on any other computer. Care should be taken that baseline and original source data files are not overwritten and that the data files for specific scenarios are descriptively named. If the input files are edited on a separate computer, they should be properly transferred to the simulation computer before executing the model so time is not used on duplicate runs. Finally, the files may also be edited with a spreadsheet program; however, they should maintain the .DAT filename extension and no additional formatting should be included. A text editor is recommended for editing input files to avoid formatting problems that can arise when using spreadsheet software. Below is a detailed description of the header file and the three data files and their information fields. Note that each file also includes header comments describing its function and format.

XI.A PARAMETERS.H

PARAMETERS.H is the input file that specifies many of the constant values used in (and must therefore be coordinated among) the remaining data files and the processes and subroutines that comprise TEMPLES. It is important to verify that the values specified in this file not only properly reflect the desired scenario but are also referenced consistently during development of the remaining data files. In the descriptions of the other files that follow, any required specifications in PARAMETERS.H will be specifically noted to maintain awareness of the necessary consistency.

The major definitions within the file PARAMETERS.H are:

JSRC: *The number of source types*

TEMPLES/CMAQ assumes that only Area, Point, and Mobile sources are of interest to the user. However, other source types (biogenic, fire, etc...) are accommodated by CMAQ and if these are of interest (note that they are still included in TEMPLES/CMAQ, simply not considered variables), then JSRC would need to be modified to define the size of the pertinent vectors, matrices, and required data definitions.

KSCC: *The total number of Standard Classification Codes (SCC) among all source types.*

ITECA, ITECM, ITECP: *The number of technologies for each source type.*

For example, for (A)rea sources of a prospective scenario, there may be 6 technologies under consideration, all for residential use: cooktops, ovens, broilers, furnaces, tankless water heaters, and storage water heaters. Thus, ITECA would be 6. TEMPLES/CMAQ only considers (A)rea, (M)obile, and (P)oint sources. These values define the expected length of data sets, especially the emission values for each technology.

KASCC,KMSCC,KPSCC: *The number of SCC codes per source type.*

The number of technologies and the number of SCC codes do not have to be equal. TEMPLES is the interface between standardized emissions data on regional and state levels and individual burner emissions data. The correlation between the two is handled in XREF_TABLE.DAT. Thus, the user is free to specify data according to these classification methods independently in PARAMETERS.H.

LPOL: *The number of pollutant species considered by TEMPLES/CMAQ.*

Currently, there are only five species considered and the structure of the input data is built on this assumption. The species (in order of their data declarations throughout the code files) are nitrogen oxides (NO_x), carbon monoxide (CO), sulphur oxides (SO_x), volatile organic compounds (VOC), and particulate matter smaller than 2.5 microns PM_{2.5}.

MLOC: *The number of counties in California, 58 as of March 2013.*

This is most directly used to specify spatial variation in natural gas properties. It also allows output data to be provided on a per-county basis.

Following these variable declarations in PARAMETERS.H (see Figure 1) is the initialization of several vectors and matrices that are used throughout the model's execution. At the end of the file is a set of ordered lists, as shown in Figure 2. The first three vectors are related to the SCC codes for the included source types: ASCC, MSCC, and PSCC. The lengths of these vectors must match the variables KASCC, KMSCC, and KPSCC, respectively. Finally, the vector POL provides the names of the pollutant species considered by TEMPLES/CMAQ. Likewise, the number of entries in this vector must be equal to the value specified in LPOL.

```

INTEGER ITECH, JSRC, KSCC, LPOL, MLOC
INTEGER ITECA, ITECM, ITECP
INTEGER KASCC, KMSCC, KPSCC
INTEGER I, J, K, L, M
INTEGER ILOC
INTEGER IKASCC, IKMSCC, IKPSCC

PARAMETER (ITECH = 40, ! NUMBER OF TECHNOLOGIES ANALYZED IN LAB EXPERIMENTS, LITERATURE
& JSRC = 3, ! NUMBER OF SOURCE TYPES: AREA, POINT, MOBILE
& KSCC = 100, ! NUMBER OF SCC CODES
& ITECA = 8, ! NUMBER OF TECHNOLOGIES ANALYZED IN LAB EXPERIMENTS, LITERATURE FOR AREA SOURCES
& ITECM = 1, ! NUMBER OF TECHNOLOGIES ANALYZED IN LAB EXPERIMENTS, LITERATURE FOR MOBILE SOURCES
& ITECP = 2, ! NUMBER OF TECHNOLOGIES ANALYZED IN LAB EXPERIMENTS, LITERATURE FOR POINT SOURCES
& KASCC = 7, ! NUMBER OF SCC CODES FOR AREA SOURCE
& KPSCC = 28, ! NUMBER OF SCC CODES FOR POINT SOURCES
& KMSCC = 5, ! NUMBER OF SCC CODES FOR MOBILE SOURCES
& LPOL = 5, ! NUMBER OF POLLUTANTS: NOX, CO, SOX, VOC, PM
& MLOC = 58) ! NUMBER OF COUNTIES

REAL EA(ITECA,LPOL), ! EMISSION FACTOR PER TECHNOLOGY (GRAMS/JOULE)
& EM(ITECM,LPOL), ! EMISSION FACTOR PER TECHNOLOGY (GRAMS/JOULE)
& EP(ITECP,LPOL), ! EMISSION FACTOR PER TECHNOLOGY (GRAMS/JOULE)
& DEDWIA(ITECA,LPOL), ! EMISSION INCREASE PER 50 BTU/SCF INCREASE IN WOBBE INDEX (GRAMS/JOULE)
& DEDWIM(ITECM,LPOL), ! EMISSION INCREASE PER 50 BTU/SCF INCREASE IN WOBBE INDEX (GRAMS/JOULE)
& DEDWIP(ITECP,LPOL), ! EMISSION INCREASE PER 50 BTU/SCF INCREASE IN WOBBE INDEX (GRAMS/JOULE)
& NDEDWIA(ITECA,LPOL), ! NORMALIZED EMISSION INCREASE PER 50 BTU/SCF INCREASE IN WOBBE INDEX (DIMENSIONLESS)
& NDEDWIM(ITECM,LPOL), ! NORMALIZED EMISSION INCREASE PER 50 BTU/SCF INCREASE IN WOBBE INDEX (DIMENSIONLESS)
& NDEDWIP(ITECP,LPOL), ! NORMALIZED EMISSION INCREASE PER 50 BTU/SCF INCREASE IN WOBBE INDEX (DIMENSIONLESS)
& XREFA(ITECA,KASCC), ! CROSS-REFERENCE BETWEEN TECHNOLOGY AND SCC CODES DISAGGREGATED FOR AREA SOURCES
& XREFP(ITECP,KPSCC), ! CROSS-REFERENCE BETWEEN TECHNOLOGY AND SCC CODES DISAGGREGATED FOR POINT SOURCES
& XREFM(ITECM,KMSCC), ! CROSS-REFERENCE BETWEEN TECHNOLOGY AND SCC CODES DISAGGREGATED FOR MOBILE SOURCES
& BE(JSRC,KSCC,LPOL,MLOC), ! BASELINE EMISSIONS IN THE INVENTORY, COUNTY-WIDE (KG/DAY)
& IE(JSRC,KSCC,LPOL,MLOC), ! INCREASE IN EMISSIONS DUE TO CHANGE IN WOBBE (KG/DAY)
& NIEA(KASCC,LPOL,MLOC), ! NORMALIZED INCREASE IN EMISSIONS DUE TO CHANGE IN WOBBE (DIMENSIONLESS)
& NIEM(KMSCC,LPOL,MLOC), ! NORMALIZED INCREASE IN EMISSIONS DUE TO CHANGE IN WOBBE (DIMENSIONLESS)
& NIEP(KPSCC,LPOL,MLOC), ! NORMALIZED INCREASE IN EMISSIONS DUE TO CHANGE IN WOBBE (DIMENSIONLESS)
& DWI(MLOC) ! CHANGE IN WOBBE INDEX PER COUNTY

CHARACTER SCC(KSCC)*10, ASCC(KASCC)*10, PSCC(KPSCC)*8
CHARACTER MSCC(KMSCC)*10
CHARACTER POL(LPOL)*5, FIPS(MLOC)*5

```

Figure 1: PARAMETERS.H Header File

```

CHARACTER TEXT*100

DATA ASCC /'2101006000',
& '2102006000',
& '2102006002',
& '2103006000',
& '2104006000',
& '2104006010',
& '2310020000'/

DATA MSCC /'2268000000',
& '2268003020',
& '2268006005',
& '2268006020',
& '2268008005'/

DATA PSCC /'10100601',
& '10100602',
& '10100604',
& '10200601',
& '10200602',
& '10200603',
& '10200604',
& '10300601',
& '10300602',
& '10300603',
& '20100201',
& '20100202',
& '20100205',
& '20200201',
& '20200202',
& '20200203',
& '20200204',
& '20200205',
& '20200252',
& '20200253',
& '20200254',
& '20300201',
& '20300202',
& '20300203',
& '20300204',
& '39000602',
& '39000603',
& '39000699'/

DATA POL /'NOX ',
& 'CO ',
& 'SO2 ',
& 'VOC ',
& 'PM2_5'/

```

Figure 2: PARAMETERS.H Header File, cont'd.

XI.B MEASUREMENTS.DAT

The file MEASUREMENTS.DAT specifies the emission rate factors used in TEMPLES/CMAQ simulations for the species NO_x, CO, SO_x, VOC, and PM. Emission rate factors are further provided for all technologies that will be considered for a given scenario. Specification of the values within MEASUREMENTS.DAT is highly dependent on prior work from the user. Appropriate, reliable, and well-supported values for the baseline emissions and emissions changes of each pollutant species for each technology must be identified. Care should be taken to properly specify the range of technologies under consideration to meet the user's goals. Two types of emissions rate factors are specified within the file:

1. *Baseline emission rate factors for each technology and pollutant species, in units of nanograms of emitted species per Joule of fuel heating value.*

This is based on an assumed (or demonstrated) baseline fuel composition with a set WI and heating value. The user must be consistent on the choice of LHV for a given simulation.

2. *Change in emission rate factors for each technology and pollutant species due to changes in natural gas fuel composition, in units of nanograms of emitted species per Joule of fuel heating value, per change of 50 BTU/scf of WI.*

The changes in fuel are specified within TEMPLES/CMAQ via the changes in WI and LHV. These units were selected because most experimental literature presents data in these same units.

Most simulations will require specification of these emission rates in absolute terms, using the real expected values. Performing a comparative study where these emission rate factors are specified only in relative terms is also possible. In this case, the baseline emissions values would all be assigned a value of 1, and changes in emissions would be specified as multiples or fractions of the base rate, still adhering to the unit specification of changes per 50 BTU/scf of WI.

The user should maintain consistency between this file and data specified in other files. First, the same number of technologies and pollutant species should be specified in the baseline emissions data and the emissions change data. Within MEASUREMENTS.DAT, the two emission rate factors are specified in blocks that immediately follow each other with no line break in between (baseline first, changes second) as shown in Figure 3. Additionally, within each of these blocks, the technologies should be arranged in order of Area sources first, followed by Mobile sources, and finally Point sources. For each of these source types, the same number of technologies should be specified in base and emissions change data, and these numbers must

reflect the values stored in ITECA, ITECM and ITECP of PARAMETERS.H. Thus, there should be the same number of lines in each block, since each technology is on a separate line. Additionally, there must be an entry for all pollutant species (the number of which is specified by LPOL in PARAMETERS.H and is usually five) in the order that they appear in the vector POL of PARAMETERS.H. If there is no data for a pollutant species (either its baseline or change value is unknown), then a value of -1 should be inserted as a placeholder. If the baseline emission rate factor for a species and technology pair is -1, then its change in emission rate factor should also be -1. TEMPLES assumes that emissions of this pollutant species are not affected by changes in gas composition for that technology.

```

# This file contains measurement data from laboratory experiments that tested emission changes due to changes in Wobbe index
# The structure is as follows:
# 1) Baseline emission factors
# 1.1) Emission factors for each technology assumed for area sources
# 1.2) Emission factors for each technology assumed for mobile sources
# 1.3) Emission factors for each technology assumed for point sources
# 2) Change in emissions due to an increase in Wobbe index of 50 Btu/scf
# 2.1) Change for each technology assumed for area sources
# 2.2) Change for each technology assumed for mobile sources
# 2.3) Change for each technology assumed for point sources
#
# Note 1: the values of emissions and emission changes can be expressed as absolute factors, e.g. ng/J, or as relative factors, in fractions. In the second case the baseline emissions would always be 1.
#
# Note 2: The number of technologies for each type of sources need to be consistent between (1) baseline values and (2) change in emissions.
#
# Note 3: The number of technologies must agree with the parameters in 'parameters.h'.
#
# Note 4: The order in pollutants is as follows: 1. NOX, 2. CO, 3. SOX, 4. VOC, 5. PM
#
# Note 5: If baseline values are not available, values are denoted by -1
#
# Note 6: Start records immediately after the last line with the '#' sign. Namely, do not leave any blank line between the headings indicated by '#' and the first record, and do not leave any blank line
#
27 14 -1 -1 -1 ! Area - Furnace
25 0 -1 -1 -1 ! Area - Storage Water Heater
20 112 -1 -1 -1 ! Area - Tankless Water Heater
35 125 -1 -1 -1 ! Area - Cooktop Burner
34 130 -1 -1 -1 ! Area - Oven Bottom Burner
29 110 -1 -1 -1 ! Area - Broiler Burner
1 -1 -1 -1 -1 ! Area - Low-NOX Burner
1 -1 -1 -1 -1 ! Area - Ultra-low-NOX Burner
-1 -1 -1 -1 -1 ! Mobile - Dummy, placeholder
1 -1 -1 -1 -1 ! Point - Low-NOX Burner
1 -1 -1 -1 -1 ! Point - Ultra-low-NOX Burner
1 -1 -1 -1 -1 ! Area - Furnace
0.2 0 -1 -1 -1 ! Area - Storage Water Heater
3 85 -1 -1 -1 ! Area - Tankless Water Heater
0.5 20 -1 -1 -1 ! Area - Cooktop Burner
-0.5 15 -1 -1 -1 ! Area - Oven Bottom Burner
1 13 -1 -1 -1 ! Area - Broiler Burner
0.4 -1 -1 -1 -1 ! Area - Low-NOX Burner
0.15 -1 -1 -1 -1 ! Area - Ultra-low-NOX Burner
-1 -1 -1 -1 -1 ! Mobile - Dummy, placeholder
0.4 -1 -1 -1 -1 ! Point - Low-NOX Burner
0.15 -1 -1 -1 -1 ! Point - Ultra-low-NOX Burner

```

Figure 3: MEASUREMENTS.DAT Sample File

Therefore, after the header information that documents MEASUREMENTS.DAT, there should be a number of entries equal to two times the number of technologies (which is equal to the sum of ITECA + ITECM + ITECP). Each line should then have a number of specified data columns equal to LPOL. The default file provided with the TEMPLES distribution includes a comment at the end each line specifying the source type and technology associated with that line's data. These comments help with bookkeeping and self-guided exploration of the input files during the learning process; it is good practice to continue this habit with further development. From the comments in the sample file, the consistent technology order in baseline emission rate factors and emission rate factor changes is apparent.

XI.C WOBBEINDEX.DAT

This file specifies the spatial variation in the natural gas fuel source according to the desired scenario. There are only two sets of information required for this data file:

1. The Federal Information Processing Standard (FIPS) code for each county in California
2. The change in WI for natural gas within each county, as specified by the user.

Thus, this data file is simply two columns of data, as shown in Figure 4. On each line, the first column is the FIPS code for a county and the second column is the expected increase in WI for that county (note the assumed direction of the change in WI). The number of rows in the data set must be equal to the value stored in MLOC of PARAMETERS.H. Additionally, the default file provided with the TEMPLES distribution includes a comment on each line with the name of the county associated with the FIPS code.

```
# Increase in Wobbe index per county
# Increase expressed in BTU/scf
# Note 6: Start records immediately after the last line with the '#' sign.
#         Namely, do not leave any blank line between the headings indicated by '#' and the
#         first record, and do not leave any blank line
#
06001 25 ! Alameda
06003 25 ! Alpine
06005 25 ! Amador
06007 25 ! Butte
06009 25 ! Calaveras
06011 25 ! Colusa
06013 25 ! Contra Costa
06015 25 ! Del Norte
06017 25 ! El Dorado
06019 25 ! Fresno
06021 25 ! Glenn
06023 25 ! Humboldt
06025 25 ! Imperial
06027 25 ! Inyo
06029 25 ! Kern
06031 25 ! Kings
06033 25 ! Lake
06035 25 ! Lassen
06037 25 ! Los Angeles
06039 25 ! Madera
06041 25 ! Marin
06043 25 ! Mariposa
06045 25 ! Mendocino
06047 25 ! Merced
06049 25 ! Modoc
06051 25 ! Mono
06053 25 ! Monterey
06055 25 ! Napa
06057 25 ! Nevada
06059 25 ! Orange
06061 25 ! Placer
06063 25 ! Plumas
06065 25 ! Riverside
06067 25 ! Sacramento
06069 25 ! San Benito
06071 25 ! San Bernardino
06073 25 ! San Diego
06075 25 ! San Francisco
06077 25 ! San Joaquin
06079 25 ! San Luis Obispo
06081 25 ! San Mateo
06083 25 ! Santa Barbara
06085 25 ! Santa Clara
06087 25 ! Santa Cruz
06089 25 ! Shasta
```

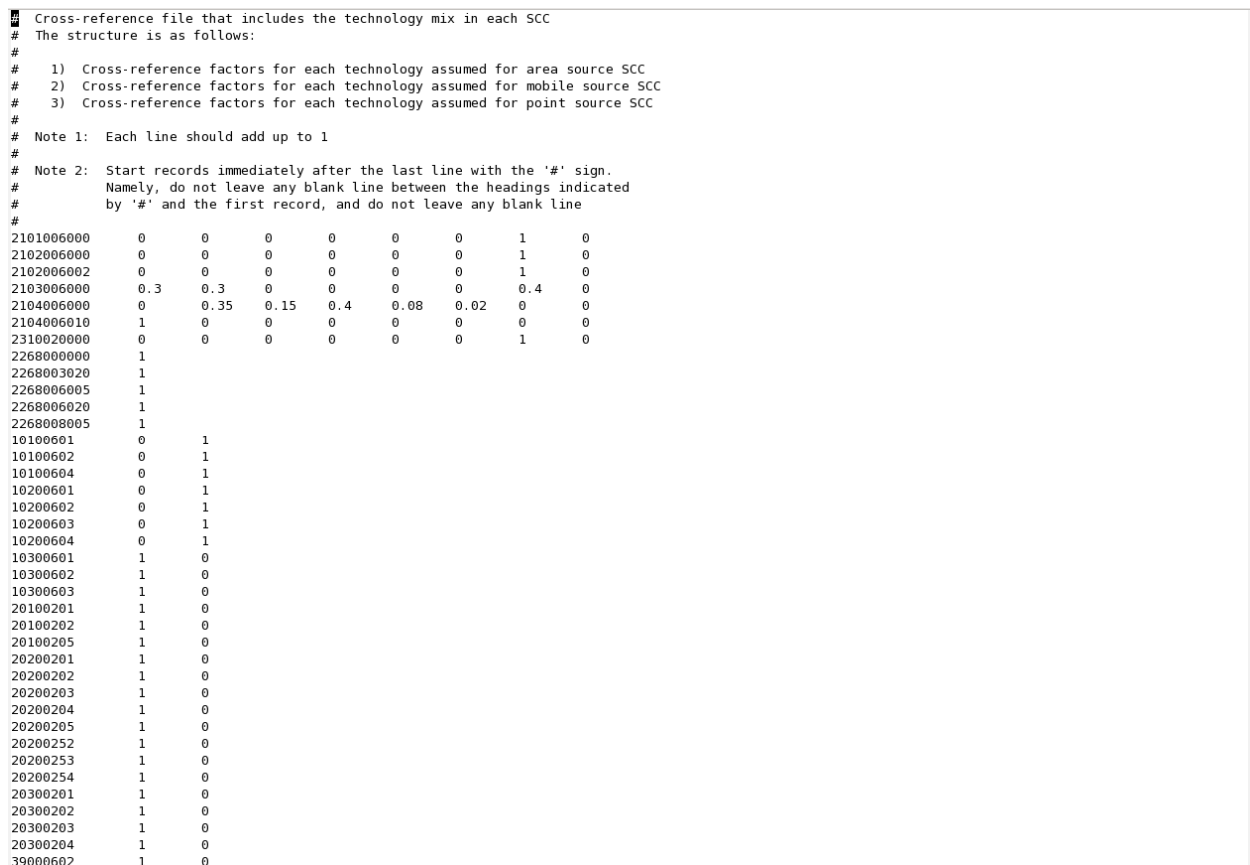
Figure 4: WOBBEINDEX.DAT Sample File

XI.D XREF_TABLE.DAT

XREF_TABLE.DAT translates information between the technology-dependent burner level and the SCC code technology groupings level. It works hand-in-hand with the emission rate factors in MEASUREMENTS.DAT and information from the National Emissions Inventory (NEI) (maintained by the federal EPA at <http://www.epa.gov/ttn/chief/eiinformation.html>) and integrated into the definitions provided to PARAMETERS.H. The necessity for this coordination arises from the expectation that the user will have access to emissions information on a more detailed level than the NEI. For example, a given SCC code may represent the total from all natural gas boilers and internal combustion engines from institutional point sources. However, this represents a broad range of technologies, each of which has different emissions responses to changes in WI. If the technology-specific level of detail is available to the user, then there must be a specification for

how each of these technologies proportionally contributes to the total specified by the SCC code. The data of XREF_TABLE.DAT is the basis for making this calculation within TEMPLES, which must provide emissions to SMOKE and CMAQ according to the broad SCC definitions.

The main goal of XREF_TABLE.DAT is to specify the contribution for each of the user-defined types of technologies within each source type to the overall definition of the related SCC code(s). As with the previously discussed files, XREF_TABLE.DAT assumes the three standard source types: Area, Mobile, and Point sources. The file is three tables of data consecutively listed after the headers, one table each for Area, Mobile and Point sources, in that order. Figure 5 displays the format; the Area sources table is SCC codes 20101006000 through 2268008005; the Mobile sources table is SCC codes 2268000000 through 2268008005; the Point sources table is codes 10100601 through the end of the file.



```

# Cross-reference file that includes the technology mix in each SCC
# The structure is as follows:
#
# 1) Cross-reference factors for each technology assumed for area source SCC
# 2) Cross-reference factors for each technology assumed for mobile source SCC
# 3) Cross-reference factors for each technology assumed for point source SCC
#
# Note 1: Each line should add up to 1
#
# Note 2: Start records immediately after the last line with the '#' sign.
# Namely, do not leave any blank line between the headings indicated
# by '#' and the first record, and do not leave any blank line
#
2101006000 0 0 0 0 0 0 1 0
2102006000 0 0 0 0 0 0 1 0
2102006002 0 0 0 0 0 0 1 0
2103006000 0.3 0.3 0 0 0 0 0.4 0
2104006000 0 0.35 0.15 0.4 0.08 0.02 0 0
2104006010 1 0 0 0 0 0 0 0
2310020000 0 0 0 0 0 0 1 0
2268000000 1
2268003020 1
2268006005 1
2268006020 1
2268008005 1
10100601 0 1
10100602 0 1
10100604 0 1
10200601 0 1
10200602 0 1
10200603 0 1
10200604 0 1
10300601 1 0
10300602 1 0
10300603 1 0
20100201 1 0
20100202 1 0
20100205 1 0
20200201 1 0
20200202 1 0
20200203 1 0
20200204 1 0
20200205 1 0
20200252 1 0
20200253 1 0
20200254 1 0
20300201 1 0
20300202 1 0
20300203 1 0
20300204 1 0
39000602 1 0

```

Figure 5: XREF_TABLE.DAT Sample File

Within each source type table, the entries specify the proportional representation of each technology for the SCC code. Each line begins with an SCC code associated with the appropriate source type. Within each source type's table, the number of lines should be equal to KASCC, KMSSC or KPSSC (whichever is appropriate) and the contents of the lines should match the entries in the vector ASCC, MSSC or PSSC, all of which are defined in PARAMETERS.H. The number of columns for each source type table should be equal to ITECA, ITECM, or ITECP plus one for the SCC code. Thus, a cross-reference is established for a pair of SCC and technology type as defined

by the column and row indices within a table. For example, if KASCC is set to six and ITECA is set to five, then the first table in the file should have six rows (with the first column matching the entries of ASCC) and six columns (one for SCC code and one for each of the five area source technologies). Since the definition of the cross-reference table is treated on a proportional basis, the entries in the columns after the SCC should sum to one. Thus, following the previous example, if each of the five technologies is equally represented within the broad category defined by the first SCC code, then each of the five entries would be set to 0.2. If a technology is not a part of the population related to a given SCC code, then it should have a zero for its entry. There should always be ITECA, ITECM, or ITECP values explicitly defined for each SCC code in the appropriate source type table.

XI.E SETPROGRAM

Finally, SETPROGRAM serves two purposes:

1. *To set the location of the netCDF library path.*

The exact location of this path depends on the decisions made during the installation phase. The library path variable, LD_LIBRARY_PATH, should be set equal to \$LD_LIBRARY_PATH:/<path to the directory where netCDF is installed>/lib/. The full specification of the path should be verified by manual inspection - navigation with the **cd** command and listing of directory contents with the **ls** command. If errors related to netCDF are encountered during the compilation or running of TEMPLES/CMAQ then it is likely that this library path has not been properly defined.

2. *To set the location of the TEMPLES-related files.*

The variable EPHOME should be set equal to <path to the directory where TEMPLES was installed>/EMPROC. Again, this directory path should be verified manually.

XII Running TEMPLES/CMAQ

Once all the input files described above are modified with the appropriate data for a desired scenario, running the simulation requires only two steps. First the definitions in SETPROGRAM must be loaded into the computer's memory so these values can be used by the remaining scripts and codes that comprise TEMPLES/CMAQ. To load the two definitions in SETPROGRAM into the session memory, the user must first start a terminal program. In Ubuntu/Linux, this can be accessed by clicking the Ubuntu logo and typing **terminal**. Once in the terminal program, navigate to the TEMPLES/CMAQ installation folder using the **cd** command. This folder may contain other subfolders for the supporting libraries and utilities that are referenced by CMAQ and TEMPLES; it will at least contain the folder EMPROC that is required for TEMPLES operation. This folder should also contain the file SETPROGRAM. Once in the installation folder, the values within SETPROGRAM can be loaded by typing:

> source setprogram

After this, navigate to EMPROC.SH. Execute the model run and save the output data to uniquely-named descriptive files by typing:

> EMPROC.sh <run-name>

This will execute the simulation, starting with TEMPLES and eventually CMAQ. During execution, several messages scroll by on the screen (often quickly). As long as the messages continue and no warnings or error messages occur, then the model code is executing properly. On the hardware at University of California, Irvine, each phase of the execution requires the following approximate times:

- Reading inputs: ~3 minutes
- Generating model-ready emissions: ~25 minutes
- Simulating air quality: ~8 hours

XIII Overview of Output Files

Upon executing the TEMPLES/CMAQ model, a set of data files will be created within the working directory. Some are intermediate emissions files written by TEMPLES and used as input for CMAQ, some are the same data, but presented in a format useful for later visualization, and still others are the final results from CMAQ. The locations and descriptions of these output files are described below.

Once the model completes execution, the folder with EMPROC.SH will contain several newlycreated files. These are all the intermediate data files for the development of spatially and temporally resolved emissions, formatted to act as input data for CMAQ. Assuming that the name provided for the test case was "Case1", the following files should be visible in the folder:

- GCNTL_AREA_Case1.TXT
- GCNTL_POINT_Case1.TXT
- GCNTL_MOBILE_Case1.TXT
- cntl_Case1_nonpt_NG_CA_orl.txt
- cntl_Case1_nonroad_NG_CA_orl.txt
- cntl_Case1_ptipm_NG_CA_orl.txt
- cntl_Case1_ptday_cem_NG_jul_ida.txt
- cntl_Case1_ptday_noncem_NG_jul_ida.txt

- cntl_Case1_ptnonipm_NG_CA_orl.txt
- cntl_Case1_ptday_cem_NG_30jun_ida.txt
- cntl_Case1_ptday_noncem_NG_30jun_ida.txt

If these files do not all appear in the folder, then an error occurred during model execution. These files are not of direct utility to the user, but part of the verification process for a successful run should include a check that these files have been updated as a result of the latest simulation.

Within this same working folder, there should also be two subfolders: EMIS and cctm. The folder EMIS contains both netCDF data files for visualizing emissions and air quality and text files that summarize emissions data from the simulation. These files are the primary output of TEMPLES and SMOKE and part of the primary input to CMAQ. The netCDF file names will have the following format:

- emis_lng_scenario_4CA_<Simulation_Date>_Case1.ncf

The folder should contain one netCDF file for each day spanned by the simulation. The files should be in chronological order from the initial date simulated to the final date simulated, without any gaps. Typically, seven days of air quality will be simulated, and there should be seven corresponding netCDF files in the folder. These files can be viewed using VERDI software, which allows the user to generate still-image or animated contour maps of the spatially-and-temporally resolved emissions. Refer to Section XV for further information on viewing these files in VERDI.

The text files that should be present in this folder are:

- AVERAGE_EMISSIONS_PER_COUNTY_Case1.txt
- JULY_EMISSIONS_PER_COUNTY_Case1.txt
- AVERAGE_EMISSIONS_PER_SCC_Case1.txt
- JULY_EMISSIONS_PER_SCC_Case1.txt

Within these files, data are provided according to two different levels of division and based on two different durations of averaging. For files beginning with AVERAGE, tables of data for the yearlyaveraged daily emissions values (tons per day) of the species CO, NO_x, VOC, PM₁₀, PM_{2.5}, PM_C, SO₂, and NH₃ are presented. In the files beginning with JULY, the same data are provided but they are the specific monthly averages for the scenario's simulated month. Thus, the data in the JULY files more directly correspond to the input information for the particular simulation just completed. In the PER_COUNTY files, pollutant emissions are summed across all SCC codes; the values in the table are thus yearly (or monthly)-averaged daily emissions within each county for each of the listed pollutant species. The counties are denoted by their FIPS code, not by their names. Finally, the files that are PER_SCC break down the totals even further, providing by-county and by-species

emissions within each SCC code evaluated by TEMPLES. Thus, data are only provided for emissions from natural gas burning sources.

The second output subfolder is cctm. This folder contains the results of the CMAQ air quality simulation, all in netCDF format. After a successful simulation, the files that are present in this folder are:

- Case1.DRYDEP.<SIMULATION_DATE>.ncf
- Case1.CONC.<SIMULATION_DATE>.ncf
- Case1.WETDEP1.<SIMULATION_DATE>.ncf
- Case1.AEROVIS.<SIMULATION_DATE>.ncf
- Case1.ACONC.<SIMULATION_DATE>.ncf
- Case1.CGRID.<SIMULATION_DATE>.ncf

Although these are all simulation results, for the majority of TEMPLES/CMAQ users, the only file that will be of interest is the CONC file, as this is the file that contains all the spatially-and-temporally resolved atmospheric concentration data. For many, this will be considered the primary output of CMAQ and the entire TEMPLES/CMAQ software suite. In format and content, it is similar to the emis_lng_scenario files located in the EMIS folder (discussed above), with the difference being that the CONC file contains concentrations while emis_lng_scenario contains emission rates. Thus, the CONC file's use is similar to the process discussed for the emis_lng_scenario files and the user is referred to Section XV for further information on the utility of this file. For advanced users, the following is a brief overview of the remaining files (for those interested in the subject, it is strongly recommended that the CMAQ user's manual is referenced for further detail):

DRYDEP: *Cumulative hourly deposition rates for selected species of interest (a different subset from the set of species modified by TEMPLES) via processes that are considered "dry."*

This typically refers to gaseous species and aerosols.

WETDEP1: *Cumulative hourly deposition rates for selected species of interest (which may or may not be the same as the species considered in DRYDEP) via processes that are considered "wet."*

This also typically refers to gaseous species and aerosols.

AEROVIS: *Hourly data for calculated visibility and light scattering due to the gaseous and aerosol species in the atmosphere at the end of each time step.*

ACONC: *The hourly-averaged atmospheric concentration of all species throughout the domain.*

Values in this file differ from the values in CONC, which are only for the end-of-time-step instantaneous solution for all species concentrations.

CGRID: *Gridded information regarding the concentration field solutions from the CMAQ simulation.*

XIV Modifying Input Files to Match Scenario Definitions

In Section XI, the input file formats and guidelines for proper editing and cross-file consistency of important data values were discussed. In this section, a few remaining details for properly editing files for scenarios matching the default assumptions and structure of the data are presented. The previous description of the input files mentioned the need for full consistency among the files; these issues are of critical importance and a review of the information in Section XI is suggested prior to any modification of input files.

The input .DAT and .H files can be edited either in a standard text editor or a spreadsheet program. However, a text editor is recommended for two reasons:

- 1) The input files all contain headers which may be difficult to read when imported to a column-delimiting spreadsheet program like EXCEL. Additionally, PARAMETERS.H in particular is not in a column-based table format and therefore is not amenable to manipulation in column- and row-divided spreadsheet.
- 2) Spreadsheet editors like EXCEL can place additional formatting information into edited files. This extra formatting can make it difficult or impossible for TEMPLES/CMAQ to use the edited file.

This manual assumes that the user has used a text editor to modify the input files. Suggested text editors for manipulation within Ubuntu/Linux are Nano, Emacs, and Pico. Within a Windows system, the suggested text editors are Emacs, Word, Notepad, and Wordpad. Note that emacs is available for both Windows and Ubuntu, allowing greater flexibility to the user. Additionally, if users wish to modify the TEMPLES itself by developing their own code, Emacs is pre-loaded with features that ease editing of FORTRAN .F files.

For example, if the user opens the file MEASUREMENTS.DAT provided with the TEMPLES/CMAQ distribution within emacs, a window similar to Figure 3 should appear. Although the data are all presented in columns, due to the varying amount of digits for some data, the width of fields (and thus trailing and/or leading spaces) is variable. When reading input files, TEMPLES does not require data within a specific field of columns; rather, it simply searches for the spaces that separate the expected values. Therefore, if the user wishes to change the baseline CO emissions from the Area Source Broiler Burner to only 90 ng/J, the modification in Figure 6 would be an acceptable edit to the file (the highlighting is added only to aide in quickly identifying the change).

```
# This file contains measurement data from laboratory experiments that tested emission changes due to changes in
; Wobbe index
# The structure is as follows:
# 1) Baseline emission factors
# 1.1) Emission factors for each technology assumed for area sources
# 1.2) Emission factors for each technology assumed for mobile sources
# 1.3) Emission factors for each technology assumed for point sources
# 2) Change in emissions due to an increase in Wobbe index of 50 Btu/scf
# 2.1) Change for each technology assumed for area sources
# 2.2) Change for each technology assumed for mobile sources
# 2.3) Change for each technology assumed for point sources
#
# Note 1: the values of emissions and emission changes can be expressed as absolute factors, e.g. ng/J, or as r
relative factors, in fractions. In the second case
# the baseline emissions would always be 1.
#
# Note 2: The number of technologies for each type of sources need to be consistent between (1) baseline values
; and (2) change in emissions.
#
# Note 3: The number of technologies must agree with the parameters in 'parameters.h'.
#
# Note 4: The order in pollutants is as follows: 1. NOX, 2. CO, 3. SOX, 4. VOC, 5. PM
#
# Note 5: If baseline values are not available, values are denoted by -1
#
# Note 6: Start records immediately after the last line with the '#' sign. Namely, do not leave any blank line
; between the headings indicated by '#' and the
# first record, and do not leave any blank line
#
27 14 -1 -1 -1 ! Area - Furnace
25 0 -1 -1 -1 ! Area - Storage Water Heater
20 112 -1 -1 -1 ! Area - Tankless Water Heater
35 125 -1 -1 -1 ! Area - Cooktop Burner
34 130 -1 -1 -1 ! Area - Oven Bottom Burner
29 90 -1 -1 -1 ! Area - Broiler Burner
1 -1 -1 -1 -1 ! Area - Low-NOX Burner
1 -1 -1 -1 -1 ! Area - Ultralow-NOX Burner
-1 -1 -1 -1 -1 ! Mobile - Dummy, placeholder
1 -1 -1 -1 -1 ! Point - Low-NOX Burner
1 -1 -1 -1 -1 ! Point - Ultralow-NOX Burner
1 -1 -1 -1 -1 ! Area - Furnace
0.2 0 -1 -1 -1 ! Area - Storage Water Heater
3 85 -1 -1 -1 ! Area - Tankless Water Heater
0.5 20 -1 -1 -1 ! Area - Cooktop Burner
-0.5 15 -1 -1 -1 ! Area - Oven Bottom Burner
1 13 -1 -1 -1 ! Area - Broiler Burner
0.4 -1 -1 -1 -1 ! Area - Low-NOX Burner
0.15 -1 -1 -1 -1 ! Area - Ultralow-NOX Burner
-1 -1 -1 -1 -1 ! Mobile - Dummy, placeholder
0.4 -1 -1 -1 -1 ! Point - Low-NOX Burner
0.15 -1 -1 -1 -1 ! Point - Ultralow-NOX Burner
```

Figure 6: Modified Version of MEASUREMENTS.DAT

Alternatively, the modification in Figure 7 would also be acceptable (note the position of the datum 90 in the highlighted row):

```

# This file contains measurement data from laboratory experiments that tested emission changes due to changes in
# Wobbe index
# The structure is as follows:
# 1) Baseline emission factors
# 1.1) Emission factors for each technology assumed for area sources
# 1.2) Emission factors for each technology assumed for mobile sources
# 1.3) Emission factors for each technology assumed for point sources
# 2) Change in emissions due to an increase in Wobbe index of 50 Btu/scf
# 2.1) Change for each technology assumed for area sources
# 2.2) Change for each technology assumed for mobile sources
# 2.3) Change for each technology assumed for point sources
#
# Note 1: the values of emissions and emission changes can be expressed as absolute factors, e.g. ng/J, or as r
relative factors, in fractions. In the second case
# the baseline emissions would always be 1.
#
# Note 2: The number of technologies for each type of sources need to be consistent between (1) baseline values
and (2) change in emissions.
#
# Note 3: The number of technologies must agree with the parameters in 'parameters.h'.
#
# Note 4: The order in pollutants is as follows: 1. NOX, 2. CO, 3. SOX, 4. VOC, 5. PM
#
# Note 5: If baseline values are not available, values are denoted by -1
#
# Note 6: Start records immediately after the last line with the '#' sign. Namely, do not leave any blank line
between the headings indicated by '#' and the
# first record, and do not leave any blank line
#
27 14 -1 -1 -1 ! Area - Furnace
25 0 -1 -1 -1 ! Area - Storage Water Heater
20 112 -1 -1 -1 ! Area - Tankless Water Heater
35 125 -1 -1 -1 ! Area - Cooktop Burner
34 130 -1 -1 -1 ! Area - Oven Bottom Burner
29 90 -1 -1 -1 ! Area - Broiler Burner
1 -1 -1 -1 -1 ! Area - Low-NOX Burner
1 -1 -1 -1 -1 ! Area - Ultralow-NOX Burner
-1 -1 -1 -1 -1 ! Mobile - Dummy, placeholder
1 -1 -1 -1 -1 ! Point - Low-NOX Burner
1 -1 -1 -1 -1 ! Point - Ultralow-NOX Burner
1 -1 -1 -1 -1 ! Area - Furnace
0.2 0 -1 -1 -1 ! Area - Storage Water Heater
3 85 -1 -1 -1 ! Area - Tankless Water Heater
0.5 20 -1 -1 -1 ! Area - Cooktop Burner
-0.5 15 -1 -1 -1 ! Area - Oven Bottom Burner
1 13 -1 -1 -1 ! Area - Broiler Burner
0.4 -1 -1 -1 -1 ! Area - Low-NOX Burner
0.15 -1 -1 -1 -1 ! Area - Ultralow-NOX Burner
-1 -1 -1 -1 -1 ! Mobile - Dummy, placeholder
0.4 -1 -1 -1 -1 ! Point - Low-NOX Burner
0.15 -1 -1 -1 -1 ! Point - Ultralow-NOX Burner

```

Figure 7: Alternative Modified Version of MEASUREMENTS.DAT

Thus, while consistent space formatting between values allows for easier reading, it is not required for successful TEMPLES execution. Finally, note that comments are delimited (by default in FORTRAN) by an exclamation point; thus, the user can add any comments they wish to the lines as long as they appear after this punctuation. All of these considerations are consistent for each of the .DAT files.

The file PARAMETERS.H is a FORTRAN program header file. Thus, it is written in a convention to make it compatible with FORTRAN compilers. It is useful to have a working knowledge of some FORTRAN basics when editing this file. As a primer, a few considerations are included below:

- The first block of information with the INTEGER declarations prepare space in memory for the variables used by TEMPLES and should not be altered.

- The PARAMETER block initializes static variables that have previously been discussed. The ampersand (“&”) in the specific location of column 6 denotes a continuation from the previous line. All integer values in this block may be altered as required. Also note the use of the exclamation point to include in-line comments. Placing the letter `c` in the first column of a new line designates the entire line as a comment.
- The REAL block should not require any editing. This block simply declares the sizes of all the arrays and vectors based on the values in the PARAMETER block. Similar functionality is provided by the CHARACTER declarations.
- Specifying the length of a vector (or matrix) requires declaring the variable name followed by the dimensions in parentheses. Specifying the number of characters in a string requires following the variable name by an asterisk and the desired length. To declare a vector (or matrix) of string variables all of a given length requires first specifying the variable name, followed by the dimensions enclosed in parentheses, and finally followed by an asterisk and the length of character strings.
- All the DATA blocks treat the information as character strings, whether the values represented are characters or integers. To specify a constant character string, enclose it within single quotation marks. Even numerical SCC codes are specified by enclosing them within single quotation marks.
- Initializing the values in an array or matrix, as in the DATA blocks, requires placing the list of initial values within backslashes.
- A FORTRAN header file does not require any statements to mark the end of the file since it is merely a set of variable declarations. Similarly, saving the header file with the suffix `.H`

and beginning the related source code .F file with `INCLUDE <PARAMETER_FILE.H>` is sufficient to ensure proper integration of the declarations within a header file.

XV Visualizing TEMPLES/CMAQ Results with VERDI

The output files of TEMPLES/CMAQ are in the netCDF file format for use in data analysis and visualization software. Several options are available for post-processing netCDF files, but TEMPLES/CMAQ has been built with VERDI as the intended tool. VERDI for Windows is freely available from CMAS at the same source as CMAQ and SMOKE. It allows the user to analyze and plot simulation data on a personal computer while additional scenarios are run on the simulation computer.

VERDI provides an easy-to-use graphical user interface, but it is important to learn a few key aspects about the software to ensure its proper use. Some of the most common tasks for users of TEMPLES/CMAQ will be presented below. VERDI is a rich and feature-filled platform with functionality well-beyond these tasks. Users who wish to gain a more advanced knowledge of VERDI should review the full manual for VERDI, provided by CMAS.

XV.A Loading Data into VERDI

To begin VERDI, navigate to the start menu, scroll down to the VERDI folder, and then click on VERDI. You will be prompted whether you want VERDI to run; click “YES” to allow VERDI to load. Once VERDI loads, the screen should look similar to the following:

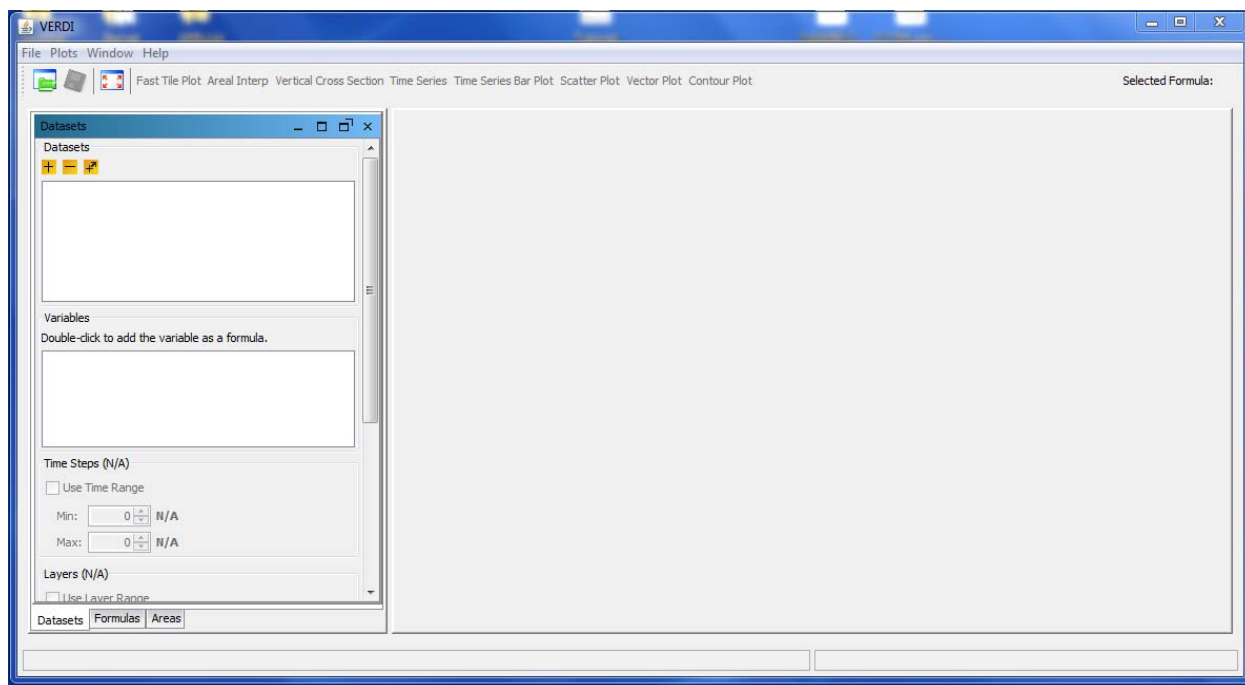


Figure 8: VERDI Startup Screen

At the top of the window is the menu bar, under which are active icon buttons for opening projects, saving projects, and unlocking (also known as undocking) windows, and a set of inactive text buttons for generating plots. At the far right is a field that reads “Selected Formula;” this will be important later when developing multiple figures from a given data set. On the left side of the window is the Datasets dialog box. Note that there are three tabs at the bottom: Datasets, Formulas, and Areas. When VERDI loads, it defaults to the Datasets tab; this guide will cover the first two tabs but leave exploration of the Areas tab to users who seek an advanced understanding of the tool.

Initially, the Datasets tab consists only of empty fields and inactive options. Loading a dataset activates these features. To load a dataset, locate the “+” (plus sign) button in the row of yellow icons immediately under the Datasets window label. Clicking this icon brings up a standard dialog box to navigate to your desired netCDF-formatted data file. Navigate to your desired output file and double-click it to open. For plotting atmospheric concentrations, the format of the filename should be <RUN_NAME>.CONC.<DATE_SIMULATED>.ncf. The selected data file will appear in the Datasets window and all pollutant species for which data were collected will be displayed in the Variables window. The Time and Layers options will now be available.

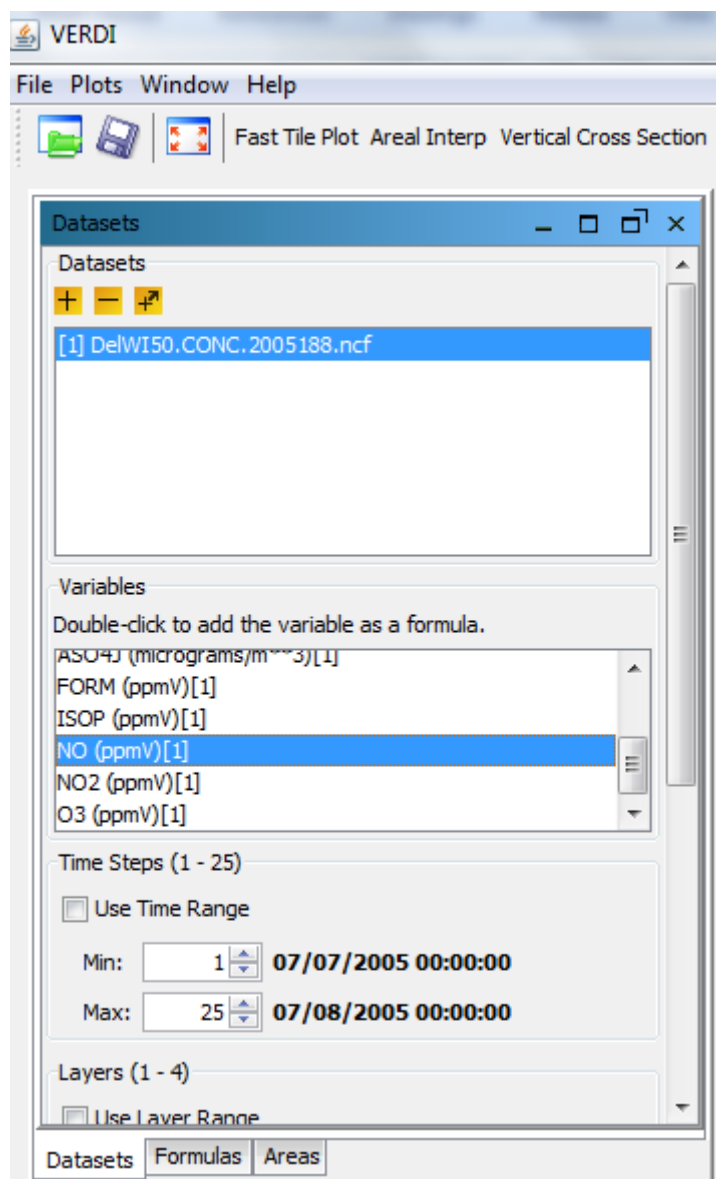


Figure 9: VERDI Datasets Panel After Loading a Dataset

To remove a dataset from VERDI, highlight it in the Datasets window and then click on the yellow “-” (minus sign) button next to the “+” button. VERDI has the capability to load multiple datasets so that differences in results between simulation scenarios can be simultaneously plotted. With one dataset already loaded into VERDI, another dataset can be loaded by clicking the “+” button, navigating to a new dataset, and double-clicking to load it. With multiple datasets loaded, the first data set will be prefaced with [1], the second with [2], and additional datasets will be numbered sequentially. It is important to keep track of the dataset associated with each index, as these will be referenced when plotting variables. The user must select the pollutant species from the correct simulation scenario to generate the desired plot, so it is helpful to give TEMPLES/CMAQ (and thus VERDI input files) descriptive names.

The options below the Variables window allow the user to plot a subset of the data. This may help focus plots on specific data, but it is not a necessary step. Pollutant concentration data from time steps and vertical layers of the atmosphere can be limited. The first option is to limit the time steps. For example, if a 24-hour period were simulated, typically there will be 25 time steps to plot. To create an animated contour plot for only a few hours in the middle of the day, the **Min** and **Max** fields can be adjusted to limit the plot to the hours between the minimum and maximum. CMAQ also simulates air quality with a vertical spatial resolution, which VERDI terms “Layers.” The dataset can be restricted by increasing the minimum layer number or decreasing the maximum layer number to focus on specific layers of the atmosphere. Layers are numbered in increasing order beginning at the land surface.

XV.B Working with Data in VERDI

When a dataset is initially loaded into VERDI, all of the available variables are listed, but none are yet activated. When variables are inactive, the “Selected Formula” field remains blank and all of the plot options are inactive. In this state, the field of formulas under the Formulas tab will also be empty. To generate a plot in VERDI, the user must first develop and select a formula.

This guide will work through developing visualizations for ozone (O_3) and NO_x (the sum of NO and NO_2) as an illustrative example. To activate a species, click on the Dataset tab and ensure that the desired dataset is highlighted (in case multiple datasets have been loaded). Next, scroll down the list of available species in the Variables window to locate your desired species. In this case, we will first choose ozone, which will typically be located near the bottom of the list. In the Variables window, the pollutant species are listed with their units (ppmV for ozone) and the index number of their dataset. Also note that even when multiple datasets are loaded, only one dataset’s variables can be actively listed and available for selection at a time. To make a species available for plotting and data extraction, highlight and double-click it in the Variables window. Upon taking this action in our example by double-clicking the entry for ozone, two changes will be apparent in the VERDI window:

- 1) The plotting options will all be active.
- 2) The “Selected Formula” field will display the selected species (“O3” in this case) and the index of its dataset.

Also, the selected species will appear at the top of the Formulas window and be available for processing. In our example, ozone would now be available for plotting. It is possible to make multiple species available for processing by returning to the Datasets tab, navigating the list of pollutant species, and double-clicking additional species. For example, to plot NO_x , it is necessary to separately add NO and NO_2 from the available species list. Keeping O_3 active, and double-clicking on NO and NO_2 will sequentially add these species to the Formulas window in the Formulas tab and update the “Selected Formula” field to the most current species.

If O₃, NO, and NO₂ have all been made available, each species will be listed in the Formulas window. In our example, ozone is displayed in units of ppmV, but standard units for ozone are ppbV. Thus, it is necessary to convert the units by creating a new formula. Modifications such as this can be achieved for any species by working in the Formulas tab. To create a new formula, with the Formulas tab open, place the cursor in the blank field to the left of the “Add” button, enter the formula (using the species name and dataset indices), and click “Add.” According to our example, to create ozone in units of ppbV, the original data needs to be multiplied by 1000. Thus, the following should be typed into the field (assuming the ozone data belongs to dataset 1):

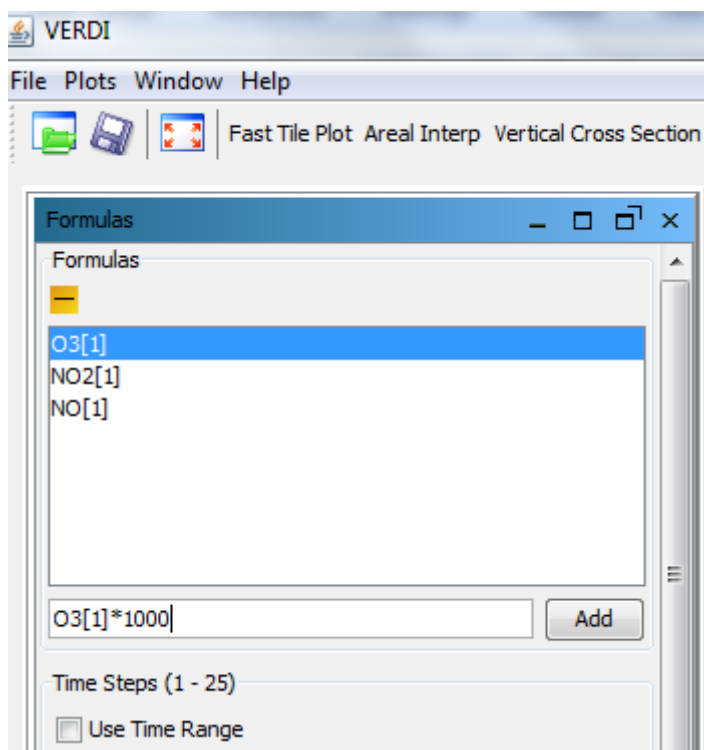
$$O3[1]*1000$$


Figure 10: VERDI Formulas Panel

Clicking the “Add” button adds this expression to the active variables in the Formulas window and this expression will become the new “selected formula.” The expression will also remain in the input field. To generate a formula for NO_x in units of ppbV, the following would be entered:

$$(NO[1]+NO2[1])*1000$$

Note that new variable names (or symbolic identifications) cannot be specified (i.e., NO and NO₂ combined cannot be renamed NO_x). If an attempt is made to create a formula with an undefined pollutant species (for example by including an incorrect index or by misspelling the variable) then a dialog box will notify the user of an error. Finally, to delete a formula, highlight it in the Formulas window and click the “-” button.

XV.C Generating Hourly Still and Animated Contour Plots

Once all of the desired species and formulas are specified and active in the Formulas window, the process of visualizing data can begin. The “Fast Tile Plot” is the most common option for generating spatially-resolved maps of species concentrations (or emissions). To create a plot for a particular species or formula, select it in the Formulas window with a click and then click the “**Fast Tile Plot**” button. The frame that dominates the right side of the program screen will fill with a contour plot of the concentration (or emission rate) of the selected formula with an overlaid map of California. In our example, completing these steps for the converted ozone in ppbV will result in the following:

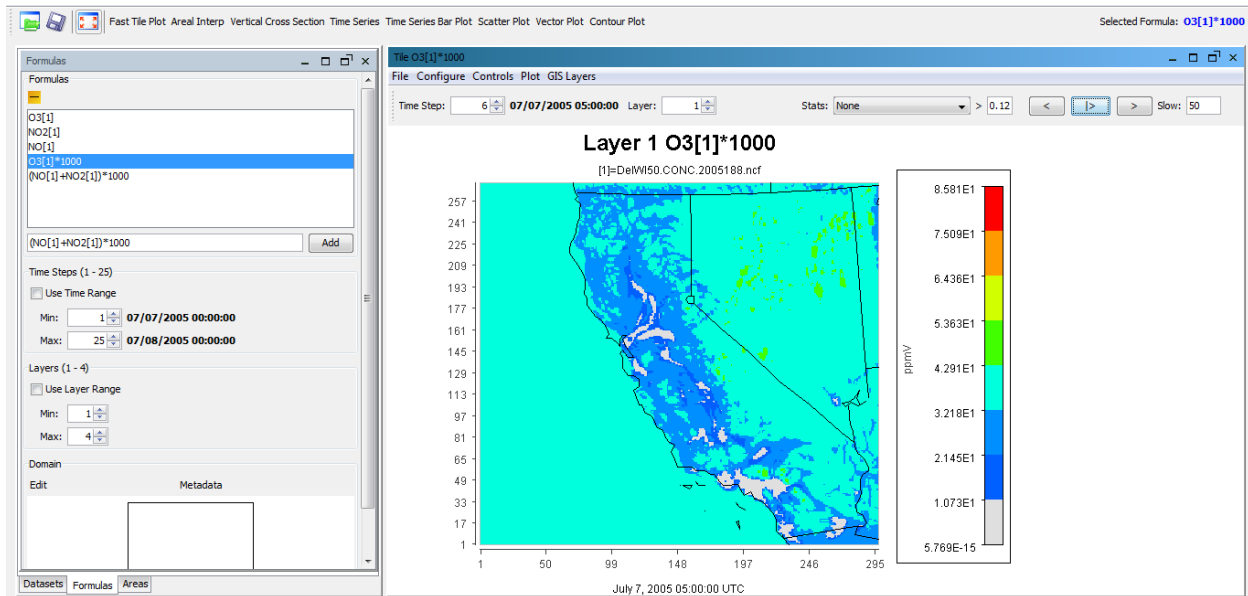


Figure 11: A Fast Tile Plot of Ozone Concentration throughout California

There are a number of considerations that require special attention at this moment. The first is that VERDI uses many default values to determine what should be plotted. As mentioned previously, there are multiple layers and time steps worth of data stored in the netCDF files that are produced by TEMPLES/CMAQ. VERDI automatically produces a map of the data in the first layer at the first time step. If this first time step is the very first solution (or even the first day of simulation), the results may not be reliable; it is best to allow dynamics from model initialization to settle before assessing predictions of atmospheric concentration. Data from the second simulation day is generally of higher quality than from the first day because the second day is less influenced by the initial conditions. The user can view data from different atmospheric layers by pressing the **up** and **down** arrows next to the “Layers” label and text box above the figure. Similarly, the control buttons above the figure and to the right move one time step back, play back all time steps as an animation, or move one time step forward. The text box next to the label “Slow” allows the user to specify the delay between animation frames, thus controlling its playback speed. Additionally, in the middle of the options above the figure is a pull-down menu to display time-averaged statistical parameters for the entire dataset.

Be aware that VERDI does not adjust its displayed units according to any of the constant factors that have been entered into the formula. Thus, while the data in our example for ozone concentration may have been adjusted to units of ppbV from ppmV, VERDI will still display the units as ppmV. This can be corrected by configuring the output figure. Clicking **Configure** in the menu bar above the figure, and then **Configure Plot**, brings up the dialog box for controlling all the adjustable parameters of the figure's display (everything other than the data itself). Clicking on the **Labels** tab at the top of the dialogue box, and then the **Legend** tab beneath that, allows the user to adjust the caption to ppbV. Clicking **Apply** will make the change without exiting the Configuration window; clicking **Ok** will make the change and exit the window.

Other display features can be configured in this dialog box including captions, fonts, and display colors. For example, the figure title bar can be renamed by clicking the **Titles** tab and providing a new title (such as "Ozone Concentration" for our example) and removing the subtitle related to the source file name. Additionally, the Color Map (and bar) can be manipulated to use a preferred set of colors or provide a smoother output image. To achieve the latter, locate the input text box next to the label "Number of Tiles" under the **Color Map** tab. By default, only 8 different colors are used for plotting. Increasing this to a larger number provides smoother gradients in the plot. The number of colors used is up to the user's discretion; however, for additional colors beyond 20, the added benefit of more colors becomes inconsequential. Also keep in mind that the data itself is not changed by these options; only the manner of displaying the data is altered.

To save a still image of a given time step, the plot must first be advanced to the desired time step using the **backward/forward** buttons at the top right. It is also good practice to verify the layer number and the "Selected Formula" before saving plots. Once the desired plot is displayed, click on the File menu option in the plot sub window (not the File menu in the upper left window of VERDI, which is for saving the entire set of work done in VERDI). Next click Export as Image/GIS. Several options for the image file type are provided. Choose the desired file type, navigate to the desired location for saving the file, give the image a descriptive name (typically based on the simulation scenario and the output species), and then click **Save**.

To save an animated plot of the species of interest, click the **Plot** menu option in the plot sub window and then click **Animate Plot**. This will bring up the Animate Plot dialog box with controls for the simulation times to be animated and for saving the animation as a .GIF, .AVI, or .MOV file (note that the available options will depend on supporting software that is installed on the user's computer). To enable these animation file formats, click on the check box next to the label "Make Animated GIF," "Make AVI," or "Make Movie," respectively. By clicking one, the user can then navigate to the desired save location and set the name of the output animation. Clicking **save** on this dialog box does not yet generate the movie. This allows the user to define one location and name for one of the movie options, return to the Animate Movie dialog box, and then set separate information for the other movie type(s) as desired. Once back at the Animate Movie dialog box with all desired information saved, click on the **Start** button to generate the specified files. The **Start** button changes to **Stop** during this process in case the user wishes to abort the process. Once the **Stop** button has reverted to **Start**, the process has completed and videos will be in the specified save location(s). It is best to leave VERDI as the focus on your desktop as the movie-making process

executes. If other applications are opened during the process, then there may be portions missing from the animation. The delay between frames cannot be manipulated when saving an animation.

XV.D Extracting Numerical Data from VERDI as Spreadsheets

In addition to visualizing data, VERDI can provide numerical data in tabulated form, though the functionality is limited. To accomplish this, VERDI includes a Probe tool so that quantitative data can be obtained quickly for a specific point or for an area on the domain. To access this tool, first ensure that the desired plot is displayed in the Plot window, then click on the **Controls** menu, and then click on the **Probe** menu option. To retrieve data for a specific point, single-click the desired location on the map. As the cursor is moved over the map, the dialog box in the bottom right of the Plot window continually updates with the grid cell of the cursor location. Thus, if the indices of the domain grid for a location are known, then data for that location can be easily obtained. Once a location is single-clicked, the text box on the bottom left of the Plot window displays the time step, vertical layer, x-axis grid index, and y-axis grid index for the selected point. . Following this location information is the value of the species of interest according to the formula that is currently plotted. Remember that the time and layer can be manipulated via the controls above the plot.

Data for a geographic region can also be obtained using the Probe tool. Click and drag on the map to delineate a rectangular area of interest. If the indices corresponding to the corners of the desired area are known, then the precision of extracting the desired area's information can be enhanced. Only a rectangular area can be selected using this method; advanced methods using shape files offer more flexibility, but these are left to the user to explore on their own with the aid of the VERDI manual. When the area selection is complete, a new window with tabulated data appears. The top row is filled by x-direction indices and the first column gives the corresponding y-axis indices. The table is filled with the values at each point for the formula that was plotted. This table can be saved for analysis in a spreadsheet application such as Excel by clicking **File** in the Plot window, choosing the **Export** option, and saving the file in .TXT or .CSV format.

Appendix B

Emission Factor Estimation in Regional Air Quality Studies of Residential Fuel Interchangeability

XVI Introduction

Simulation of air quality impacts in urban airsheds has come to be a widely-used and valuable tool in understanding the impacts of humans' activity on the environment that surrounds them. These types of investigations have come to inform not only the research community on likely causes and physical bases of observed atmospheric phenomena but have also developed to the point where they are relied upon by regulatory agencies for guidance in developing new legislation. Studies developing baseline emissions profiles given modern levels of human industry, transportation, and other activity have helped agencies determine emission reduction goals and build cases for understanding why such reductions need to be implemented. Moving forward, it is often of interest to understand and anticipate what the effects will be of scenarios that consider changes to these baseline emissions. New industry utilizing well-known equipment, phasing in and out of fuel sources, and new industry utilizing newly-developed technology are all examples of scenarios that may be of interest to regulatory agencies wishing to understand the potential impacts before they may become egregious and difficult to curtail or reverse.

Investigating the regional impact of these types of changes broadly involves three major components that must be synthesized and brought together in order to provide a meaningful and appropriately framed prediction. The first is the definition of the air quality model itself, including the development of a methodology to define the simulation domain and its geophysical features as well as the development of models of physical processes (advection, chemical reaction, diffusion, etc...) that occur within the domain. The second is the development of scenario test cases that capture the overall changes that are the focus of the investigation. This can be specified in the form of reductions in emission factors due to the introduction of regulation or new technology, increases in emissions due to the siting of new industry in a region, or the effect of new energy carriers within a region. Finally, the emissions factors for the known energy conversion devices in the region must be detailed throughout the region of interest.

The current work focuses on the last of these three aspects. In the most ideal case, an investigator could have an indexed list of all energy conversion devices in the region, and their known (averaged or representative) emission rates for all species of interest. For example, within the region of interest, the sum of all home hot water heaters' CO emissions within each node of the simulation domain could be specified. This is however not the reality. More typically, especially for devices

within the residential sector, estimates must be made based simply on assumptions of the type and number of burners within a given simulation node. The bases for the estimates include demographic and land use information as well as available emissions rates based solely on the classification of the burner. Without knowledge of the exact make and model of each device in each home, this is the best estimate available.

However, quantifying the emission factor, even for an individual specie generated by a device of a single classification, is often difficult. This is especially true when there is a desire to consider off-design operation. The current work investigates the particular case of natural gas interchangeability, developing a methodology for estimating the changes in emission factors as the composition of the regional natural gas supply is altered from the baseline case to which the devices are likely to be adjusted. Such a scenario is envisioned within the Southern California Air Basin, where an introduction of Liquefied Natural Gas (LNG) within the region will alter the composition of the natural gas arriving at the customers' locations.

XVII Background

Gas interchangeability, as defined by the Gas Interchangeability Task Group, is "the ability to substitute one gaseous fuel for another in a combustion application without materially changing operational safety, efficiency, performance or materially increasing air pollutant emissions" [1]. This task group was established by the Natural Gas Council in 2004 primarily in response to forecast changes in domestic gas compositions resulting from anticipated imports of LNG. This definition implicitly specifies interchangeability parameters and criteria as they relate to appliances in end-use. Interchangeability indices and the limits upon them are specifically based on testing conducted on appliances after manufacturing and installation. Definitions created in such a manner allow for assurance that the interchangeability limits apply to a wide range of end-use scenarios and configurations. Historically, the focus of interchangeability tests has been devoted largely to residential appliances, due to the fact that residential consumers account for a large percentage of total US natural gas consumers [2,3].

The major combustion-related concerns focus on safety, performance reliability, and appliance and equipment durability [2]. Safety concerns include CO generation in vented and unvented appliances and equipment, overheating of appliance surfaces, and overpressures due to delayed ignition. Performance reliability concerns are related to flame stability issues: flame instability leads to outages caused by the activation of safety devices due to flame blow-off and flashback from the burner head. Finally, the most serious issues associated with durability relate to thermal degradation, fatigue of appliance components such as heat exchangers, and fouling due to soot production. Initial investigations may not reveal concerns in reliability and safety performance as these may be observable only after significant usage and component degradation, requiring experimentation over extended time periods.

Failure for a given burner type is typically determined by violation of acceptable operating emissions of three species of interest- CO, soot, and NO_x. Thus, by monitoring the emission and

concentration of these species in typical installation settings, it is possible to determine which technologies will provide safe, reliable, and durable operation. These concerns must be addressed in both unvented and vented gas appliances, accounting for the possibility of vent failure in installations. Carbon monoxide production poses a risk to the consumer because it can act as a hypoxic toxin when inhaled in high dosages; continuous, improperly ventilated emission from burners can thus lead to dangerous conditions within the consumers' own homes. The American National Standards Institute (ANSI) certifies safe performance of natural gas by setting limits on acceptable CO emissions. However, the index typically used to quantify acceptable performance is historically not the CO concentration itself, but the Weaver Incomplete Combustion Index, as this is based on a more easily-observable phenomenon called yellow tipping [2].

The primary cause of excessive CO production is incomplete combustion. This results from a lack of secondary air, which typically ensures complete combustion. In form and function, residential appliance burners can be considered similar to a Bunsen burner, as shown in Figure 16. In this configuration, primary air is utilized for entrainment of fuel and mixing for some length before the combustion zone. However, the oxygen concentration must be below the combustible limit of the fuel for safe operation (in order to avoid combustion within the reactant delivery pathways, known as flashback). It is worth noting that flashback may also occur when the speed of the flame in the combustoring region exceeds the flow rate of the non-reacting stream, propagating back towards the reactant inlet ports and potentially into the fuel delivery stream and system. Secondary air is then required to allow the required amount of oxidant to react with the fuel and complete the combustion process.

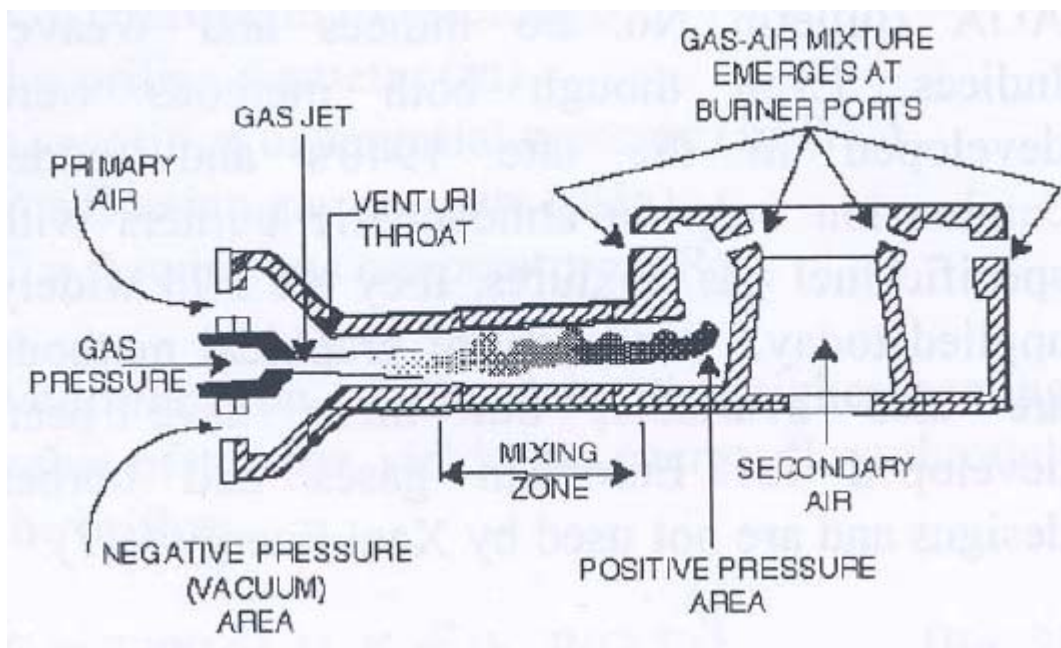
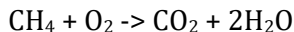


Figure 16: Typical Appliance Burner Design [4]

For the stoichiometric reaction, natural gas combustion can often be simplified for steady-state thermodynamic investigations to the reaction



However, the pathway to complete combustion is considerably more complex and consists of many sub-reactions that slowly oxidize the methane leading to formation of unstable intermediates such as methylene (CH_2), a highly reactive diradical. Primary air only causes combustion in volumes within the premixed stream where the fuel quality is high. Consequently, secondary air is required to complete the combustion. However, the methylene radicals can persist and hinder the full entrainment of oxygen, leading to increased CO formation. Furthermore, with changes in fuel composition come changes in hydrocarbon content; fuels with higher concentrations of hydrocarbons, especially hydrocarbons of higher carbon number, require more oxygen to complete the combustion. Thus, changes in the fuel composition can lead to kinetically-dominated changes in CO emission, which cannot be predicted by thermodynamic evaluation and therefore require comprehensive experimentation to properly quantify. For investigations relating to the air quality impacts and emissions of residential burners, this more complete view of natural gas combustion is necessary to achieve accurate estimation of emission impacts.

The production of soot often accompanies the production of excess CO, and is caused mainly by combustion occurring at high temperatures with low oxygen levels. Thus, the presence of insufficient oxidizer is a common factor in the production of both species. As previously noted, oxygen depletion is sensitive to the composition of the fuel being utilized; thus, CO and soot production may be directly affected by changes in available gas composition, hindering the assessment of interchangeability for a given appliance. Often times, soot may not be readily visible in the bulk flow of combustion products, given the small size of the typical particle. Additionally, soot can form in exhaust effluent from precursor species developed during combustion; thus, detection of soot becomes difficult if the sensor location is not carefully considered. Thus, soot has a tendency to accumulate over time and may lead to unsafe operating conditions in addition to adding to the total PN count in the exhaust flow. As with CO, soot is typically detected through the visual presence of yellow-tipping in the burner flame [2].

For gas appliances, NO_2 as a constituent of NO_x is a major concern in indoor environmental air quality due to its role as a respiratory irritant. More generally, NO_x emissions are not considered a primary indicator of combustor failure; however, they are a contributing factor to ozone formation, which is recognized nationally as a criteria pollutant [2]. The formation pathways and atmospheric impacts possible via NO_2 and NO_x are complex and extensive and are fairly well-understood in the current science [1]. Importantly, the United Kingdom Department of Trade and Industry determined in studies of gas interchangeability that increases in NO_x were linked to increases in the Wobbe number [5]. This correlation allows for the use of a simple, easily-calculated, composition-dependent parameter as a reliable indicator of NO_x formation, which is itself the result of varied and complex reaction mechanisms.

Table 19: AGA Flame Code Descriptions [6]

Code	Flame Description
+5	Flames lifting from ports with no flame on 25% or more of the ports
+4	Flames tend to lift from ports, but become stable after short period of operation
+3	Short inner cone, flames may be noisy
+2	Inner cones distinct and pointed
+1	Inner cones and tips distinct
0	Inner cones rounded, soft tips
-1	Inner cones visible, very soft tips
-2	Faint inner cones
-3	Inner cones broke at top, lazy wavering flames
-4	Slight yellow streaming in the outer mantles, or yellow fringes on tops of inner cones. Flames deposit no soot on impingement.
-5	Distinct yellow in outer mantles or large volumes of luminous yellow tips on inner cones. Flames deposit soot on impingement.

Traditionally, the determination of flame characteristics in residential appliance burners has relied more on visible indicators (such as the yellow tipping previously mentioned) and less on quantified measurement of parameters such as exhaust species concentrations. Thus, a more qualitative method of rating burner performance has been developed by the American Gas Association (AGA), shown in

Table 19 [6]. In addition to yellow tipping, the rating system considers the flame instability indicators of liftoff and flashback. Flame lifting is the impaired ability of a flame to stay lit, due to a higher fuel flow rate than flame speed. Factors that can contribute to such a situation include lean operation (excess oxidant), high concentration of inert species in the fuel, and increased fuel port flow rate beyond the conditions for which the burner was designed [2]. Flashback primarily becomes a concern when the fuel gas is high in hydrogen concentration. Becomes of the high flame speeds associated with hydrogen combustion, fuel mixtures containing sufficient levels of hydrogen may have a tendency for the overall flame speed to easily overcome the mass flow rate and therefore propagate the flame into the delivery system [2]. This is typically not a major concern for natural gas mixtures; however, flashback can still occur if stoichiometric conditions are achieved during primary aeration. Safe operating regions that avoid each of these undesired characteristics can be defined for each burner operating on a given fuel; Figure 17 provides an example of one such burner-and-fuel specific operating map [7].

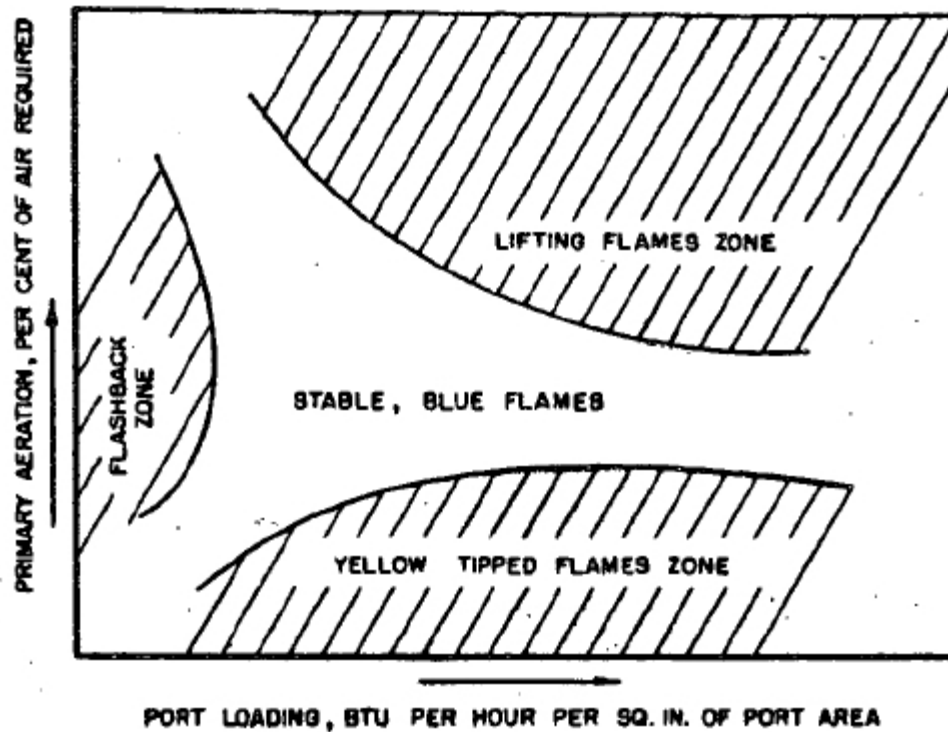


Figure 17: Burner Operating Map [7]

This method developed by the AGA is one of a few interchangeability standards currently in use. Like the AGA, the Weaver standard is based on qualitative observable indicators and provides performance standards specification that considers a wide range of critical operating parameters. However, there has additionally been substantial interest in developing correlations to more quantifiable fuel-based parameters. Currently, the Wobbe index serves as quantifiable, theoretically-based indicator of combustion performance. Defined as the ratio of fuel higher heating value to the square root of the fuel specific gravity, the Wobbe number provides a summary, but limited, measure of the fuel's heat rate delivery potential. It is important to understand that Wobbe numbers only provide context as they relate to each other or to a predefined baseline value, with care taken to ensure that sample conditions of temperature and pressure remain constant across tested fuel mixtures. In practice, the Gas Research Institute has found that Wobbe number can be a good indicator of matching burner performance if the fuel composition changes are limited [8].

Of particular importance to the current work, the Wobbe Number also plays an important role when considering LNG importation [6]. LNG supplies typically have a substantial concentration of heavier-than-methane hydrocarbons not typically found in conventional natural gases. On the other hand, these sources contain negligible amounts of CO_2 , N_2 and O_2 , which exist in California and other domestic gas supplies. Introduction of imported LNG therefore, leads to mixtures with high HHV and consequently a higher Wobbe Number. Theoretically, the correlation between Wobbe Number and the emissions composition is fairly direct. As the hydrocarbon content and composition changes, the Wobbe Number alters along with the associated heating content changes

and mixture specific gravity changes. Chemically, these changes in hydrocarbon content affect the considerations mentioned previously for the formation of CO, soot, and NO_x (and possibly other species). Thus, the Wobbe number has come to be referenced as an acceptable indicator of potential to form these species of interest.

XVIII Methodology

XVIII.A Review of LBNL Emissions Data

The emissions data analyzed in this work were reported by the Lawrence Berkeley National Laboratory in a report of experimental determination of residential appliance emissions affected by natural gas variability [9]. The experimentation was carried out on two broad groups of devices- burners utilized in cooking and preparation of food and burners integrated into space and water heaters for the home. Within these large groups were three subgroups of devices; thus the six device classifications tested were: cooktops, oven burners, broiler burners, furnaces, storage water heaters, and tankless water heaters. For each device classification, emissions data was recorded for the species CO, NO₂, NO_x, HCHO, and PM. Experiments were structured to allow investigation of a range of different fuel compositions, with the fuels' Wobbe Numbers (WN) utilized as the summary parameter to describe the fuel. Fuel WN ranged from 1320 to 1420 in the study.

Results were then presented as changes in emissions factors per change in 25 units of WN. It should be noted that inherent to this definition was the assumption on the experimenters' part that the relationship between WN and emissions was linear. Justification for this assumption and treatment of the data was presented in the original LBNL report. For all species except PM, this was given in units of ngJ⁻¹(25WN)⁻¹. PM was reported in particle number counts per 25WN. The number of units tested in each classification was not consistent; some test groups consisted of 10 or more individual units, while others consisted of 5-6 or fewer units. Multiple tests at each combination of WN and burner unit were completed in order to develop tests of statistical significance; for each combination of emission species and burner unit, a p-value for the significance of the data and an R² value for the correlation between WN and emission rate were provided. Additionally, upper and lower 95% confidence intervals (assuming a normal distribution) on the mean for each species and burner unit were provided. In most cases, bivariate statistical analysis was sufficient; there were no apparent effects on the emissions factors other than WN. In other cases, multivariate analysis was utilized in order to control for noticeable trends due to order of testing, warm-up time, and day and/or time of testing. In these cases, only p-values were provided from statistical analysis.

As presented, the emissions factors of the LBNL report provide a significant depth of detail, not only in terms of the variability within the data but also for the experimental methods and the difficulties encountered and adjustments implemented. Thus, it is worthwhile to first consider using all the data provided within each data set to develop estimates of a single representative emission factor for each species and device classification combination. A natural choice is to investigate the mean of the data and its associated confidence interval. In order to provide some discrimination of the most

significant data, critical limits of the p-value and R^2 can be implemented and only the data points that meet these criteria analyzed. For example, critical values of 0.95 for p-value and 0.9 for R^2 can be utilized to indicate a very high confidence in the resulting data. Comparing the means and ranges of the confidence intervals for all points may lead to the development of a reasonable emission factor estimate with high confidence and reliability (or at least as much as can be obtained given the small size of the data sets).

Although this method presents a theoretical possibility and is simple and elegant in application, it may present difficulties. The LBNL data utilized in this work provided a number of challenges. Figure 18 depicts three possible scenarios for this type of comparison. In the first panel, there is some amount of overlap among all the data and there is a reasonable number of applicable data; such a situation may provide an acceptable estimate. The second panel depicts a situation with some overlap, but few data points; choosing a value based on such a small subset of an already small dataset becomes difficult to justify. The final panel depicts the case with little to no consistent overlap in confidence intervals, making selection of a single value unlikely. A fourth possibility may occur, in which no data (or only one data point) meet the requirements of acceptable significance and correlation. In the analysis of the data provided by the LBNL report, these problematic scenarios appeared often and it was often required to consider loosening the critical values in order to include more than a single data point.

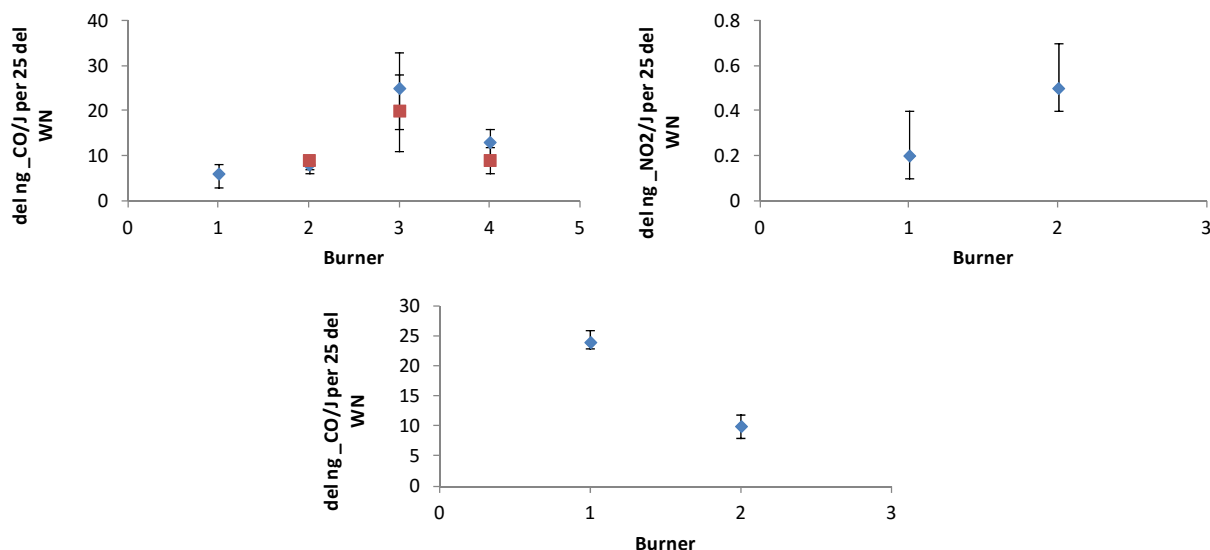


Figure 18: Possible Data Spanning Scenarios (Blue Points Indicate “Full Burn,” Red Indicated “End-of-Burn”)

Additionally, it would be desirable to find as little variability as possible across species emissions and technologies. This may not be a physical reality, but simplification of the emission factors can aid in the process of the investigator’s simulation process. Thus, if for example, NO_2 emission rates relative to WN could be found to be independent of burner type, then this would greatly simplify

the process. Such a situation may occur if the burner designs are similar across device classifications (involving such considerations as flame speed, equivalence ratio, flame length, yellow-tipping, etc...). However, analyzing the LBNL confidence interval data did not provide for this type of simplification in the data. An example comparing cooktop and broiler burners is given in Figure 19.

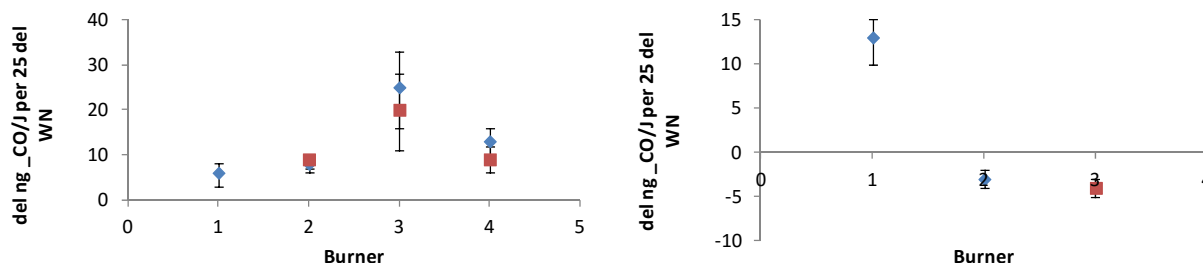


Figure 19: CO Emission Dependence on WN across Burner Types

Thus, an alternative method for analyzing the data provided is desirable. Given the small number of data points within each set, it would not be good practice to assume a normal distribution at the outset and simply set all emission factor values to the average of the data set. Indeed, inspection of the histograms for much of the data indicates that the distributions may not be normal. Thus, parametric statistical inference methods were utilized to develop a series of tests that lead to the selection of an appropriate distribution to model the data. The method developed in this work was thus created for the general case of determining emission rate factors from small amounts of supporting experimental data, which is a common situation experienced by researchers carrying out regional air quality simulations.

XVIII.B Distribution Selection

The overall goal is to identify a continuous probability distribution function with two pertinent features: 1) the distribution has a reasonable probability of being related to the observed data, and 2) the distribution has a close correlation to the observed data. Once an appropriate distribution function is selected, appropriate features of the distribution can then be utilized to develop an estimate of each required emission factor. Additionally, the method is developed in such a way that interpretations can be developed on the relative reliability of each distribution (as compared to all other candidates) as well as the absolute reliability of a chosen distribution.

The distribution candidates were chosen to be the Normal, Lognormal, Exponential, Gamma, and Weibull distributions. Each of these has 1 or 2 distribution parameters that must be identified in order to define the distribution; Minitab 16 software was employed in order to determine the

optimal distribution parameters for each distribution type. Additionally, Minitab provided two measures of the probability that the distributions were related to the observed data: the Anderson-Darling number and the p-value against the null hypothesis that the distribution shape mirrors the observed data. Both of these were recorded for each distribution for each data set along with the corresponding distribution parameter(s).

Once these parameters were obtained from Minitab, the correlation between the distributions and the observed data could be developed, satisfying the desired correlation to the observed data. The first step was to utilize the histogram from the observed data to develop the empirical cumulative distribution function. The shape parameters identified by Minitab were then utilized to calculate the cumulative distribution function for each of the candidate distributions at the values utilized as the histogram bins. A coefficient of correlation was then calculated between the empirical cumulative distribution function and each of the candidate distributions' cumulative distribution functions, following the standard definition of R^2 as 1 minus the ratio of residual sum of squares to total sum of squares.

Thus, three indicators were obtained and utilized in the selection process of the representative distribution function: the Anderson-Darling number, the p-value against the null hypothesis of the observed data following each distribution, and the correlation coefficient between each candidate distribution and the empirical cumulative probability function. It is not guaranteed that all three of these measures will be optimized by the same distribution type, and it is not guaranteed that a single distribution will clearly stand out from all other options as the optimal choice. Thus, a selection process was required for determining the optimal candidate, based on the desired features and the overall goal mentioned above.

A three-round process of determination was devised in order to assess which distribution candidate was the optimal choice, as compared to all other candidates. This portion of the overall assessment of the data therefore does not provide insight on whether or not the distributions are acceptable candidates in an absolute sense, according to strict guidelines similar to those discussed in Section XVIII.A. However, the relative comparisons allow for more flexible investigation of the merits of each distribution candidate and avoid preemptive elimination based on only a single indicator value. Moreover, the method is designed to be mechanistic and robust, so that advantages of a given distribution which may not be immediately apparent at first glance can be quantitatively captured and considered. The process of determination developed for this work was a three-round process and proceeded in the following manner:

- 1) All distributions candidates were analyzed for their AD number, p-value, and R^2 , and ranked for each indicator.
- 2) A selection was made in the first round if a single distribution candidate was associated with both the highest R^2 and either the highest p-value and/or lowest AD number among all distributions.

- 3) If no distributions could be selected in the first round, a two-step second round was initiated.
 - a. Critical indicator values were defined as being within 5% (in the optimal direction) of the best value in each indicator. (Thus, 95% of the highest p-value and R^2 and 105% of the lowest AD number.) If a single distribution candidate met these adjusted limits according to the rules of step 2, then a selection was made.
 - b. If multiple distribution candidates were able to satisfy the adjusted limits, then this subset of distributions was re-evaluated on the basis of only their indicator values. This had the possibility of then adjusting the optimal values of the indicators. If a single distribution met the requirements of step 2 based on this smaller subset of candidates then a selection was made.
- 4) If no distributions could be selected after step 3, either due to a complete lack of distributions meeting the requirements or the continuing possibility of multiple distribution candidates, then a third round selection was made simply based on the distribution with the highest average value of 1-AD, p-value, and R^2 .

Thus, the method's goal is to choose the optimal candidate among all distribution shapes on a relative basis, based on quantified measures of agreement with the basis data set. Preference is given to a selection that can be made considering all distribution choices. When this cannot be done due to multiple distributions each within partial satisfaction of the requirements, then an attempt is made to provide a selection based on the subset of distributions that appear to be most applicable after the first attempt. However, when selection is not possible either for the entire group of distributions or for a more selective subset, a determination must still be made, and the method then resorts to a simple summary rating in order to provide a final determination. As will be discussed below, each of these scenarios is not given equal consideration when a determination of the absolute effectiveness of the selected distribution is employed.

It is worth noting that any selection method (whether the one described above or an alternative) should recognize that selection of distributions other than normal (and possibly lognormal) must be supported by thoroughly-documented evidence and strong confidence in the data and

distribution selection process. Thus, whenever possible, it is desirable to build in features that will provide some preference for the normal distribution's selection. Such was the case in the method described above. The LBNL data set included many non-positive data points. Analyses of all distributions other than the Normal require these points to be removed, thus ignoring essential data and reducing the sample size. This has the effect of increasing the distribution variance and thereby negatively affecting the calculation of the p-value. In addition, it directly compromises the calculation of the coefficient of correlation for these distributions. When comparing the cumulative distribution functions, the R^2 value was calculated against the unaltered empirical cumulative distribution. Thus, at low values of the emission factors, the fit between the non-Normal distributions and the empirical data were very poor, negatively affecting the R^2 value. In some cases, this effect was so extreme as to result in large, negative R^2 , which should be interpreted as merely no demonstrable correlation for these candidate distributions. Additionally, a cap of 0.25 on the p-value of Gamma and Weibull distributions (to be discussed in Section XVIII.D) provides further limitation to the selection of these candidates in preference to the Normal. Finally once all emission factors for all device categories were determined, all the results were compared to reassess the overall likelihood that the observed data could in truth be non-normally distributed. This final summary assessment reaffirms the requirement that inferences claimed to be non-normal must come under close scrutiny.

XVIII.C Emission Factor Selection

Given the relatively large uncertainty provided by the original LBNL data, mostly due to the small number of data points and the presence of positive and negative factors within each data set, it is desirable to define a range of likely emission factor estimates. The process described in Section XVIII.B provides the estimate of what can be considered the "best engineering estimate." Once the best-fit distribution is selected, the expected value of the distribution can be selected for the best engineering estimate. Since the expected value provides the most probable value, this is a reasonable approximation for the baseline estimate. It should be noted that this is only the same as the mean for any data set where the normal distribution is determined to be the most appropriate. This is in fact the motivation for the distribution selection process, especially when one is working with data that may not appear to have a normal distribution. The reliability of the emissions estimate can be greatly improved by implementing the proper expected value of the representative distribution as opposed to the blindly applying the sample data mean.

This best estimate provides a central point for developing a baseline emissions change scenario. Upper and lower bounds that bracket this baseline value are also desirable as they can provide context for the severity of a particular emissions factor's change on the overall results of the air quality simulation. Thus, an upper-limit "maximum likely increase" and lower-limit "minimum likely increase" can be defined for the emissions factor of each species, for each device classification. A number of candidate metrics may be utilized to determine the value of these extremes. Ideally, the upper and lower bounds of a confidence interval about the expected value could be utilized to provide estimates of the range of possible expected values given the

distribution shape. However, this is only well-defined for the normal distribution and extrapolating such data from such advanced techniques as bootstrapping methods for non-normal distributions with such small data sets may be misleading in their final predictions. Thus, it is suggested that the best, consistently-applicable estimates are the 5% and 95% quantiles of the model distribution, thereby providing the bounds of 90% of the possible estimated values for a given emission factor. It is important to clearly recognize the subtle difference between the possible values described by these estimates and the most likely values provided by the expected value and its associated confidence interval.

XVIII.D Estimate of Emission Factor Reliability

Although the distribution selection process previously described allowed for the possibility of identifying the most appropriate candidate, it is not guaranteed that this distribution matches well to the original data in an absolute sense. The process described above relies only on relative comparisons among the candidate distributions. In addition, for any distribution selection made in the third and final round, the optimality of the selected distribution is more derived and less powerful than selections made in the first two rounds. It additionally provides no context for the differential impacts of a distribution's likelihood and fit indicators. Thus, in order to provide some context of the independent certainty and reliability of a given set of emission factors, the above estimates were given a "Reliability Score." The score consisted of two parts: one half of the points for the score were attributed to desired features of the observed data from the LBNL emissions measurement report and the other half were attributed to the features of the chosen distribution for each emissions specie and burner type. A total of 5 points were achievable within each category:

Sample Data Reliability Points

+1: Total number of data points (after removal of non-positive values, if appropriate) greater than or equal to 5.

+1: Total number of data points (after removal of non-positive values, if appropriate) greater than or equal to 10.

+1: p-value less than or equal to 0.1 for at least half of applicable data.

+1: R^2 greater than or equal to 0.75 for at least half of applicable data.

+1: p-value and R^2 requirements met for at least one quarter of applicable data.

("Applicable data" refers to all data that could be utilized given the chosen distribution. For normal distributions, this included all the original data in a given set. For all other distributions, non-positive data could not be included. Thus, all determinations above were then made on the basis of the smaller data set with these points removed.)

Distribution Reliability Points

+1: Anderson-Darling value of chosen distribution less than or equal to 0.35.

+1: p-value of chosen distribution greater than or equal to 0.75.

+1: R^2 value of chosen distribution greater than or equal to 0.8.

+2: Distribution identified in round 1 as previously described.

Or

+1: Distribution identified in round 2 as previously described.

(No points awarded for distribution identified in final round)

There were a couple of exceptions that had to be made for these rules. For any set of data that came from a multivariate analysis, no R^2 value was provided by the LBNL report. It was assumed that the attempt to control for secondary effects on the observed trends provided an extra measure of confidence in the results. Thus, for multivariate data, the rules for Sample Data Reliability were applied as if all data points in the set had an R^2 value above the critical point. Additionally, the Weibull and Gamma distributions do not have a closed-form analytical solution for the p-value above 0.25. Although advanced methods including computer simulation can be implemented in order to provide estimates, the data provided by Minitab does not employ these methods. Instead, an indication is simply given that the p-value exceeds this upper limit. Thus, for Weibull and Gamma distributions, the second point of the Distribution Reliability was counted if their p-values were indicated to have exceeded this limit. For the purposes of calculating the distribution's average of 1-AD, p-value, and R^2 , a value of 0.25 was used for the p-value in these cases in order to maintain a conservative estimate (giving deference to the more commonly-observed Normal, Lognormal, and Exponential distributions).

Thus, the Reliability Score provides a summarized interpretation of the degree to which the chosen distribution and the underlying data meet the larger goals of the process: namely, to provide the most appropriate estimate basis for emission factors, based on a sufficiently-sized and representative data set. The point system above did allow for some accounting of the nature of the original data sets; for example, sample sizes of 5 and 10 are very low in the context of most statistical inference. However, in the context of the limited availability of data in this particular study, these values represented reasonable limits of distribution sizes that might be considered too small and at least sufficiently large for some estimation. Similar considerations motivated the development of the critical values in the other measures. Once the Reliability Score was calculated for each pair emission specie and device classification, then a qualitative descriptor was attached with the following guidelines:

0-2: Very Low Reliability

3-4: Low Reliability

5-6: Medium Reliability

7-8: High Reliability

9-10: Very High Reliability

XIX Results

The method described in Sections XVIII.B through XVIII.D was applied to the observed data obtained from the LBNL residential burner study. For the most part, the data was considered as presented (with required exception of removing non-positive data for non-normal analyses). During analysis, it was found that one outlier data point should be removed from the NO₂ and HCHO emission results for cooktops and for the CO emission results for tankless water heaters. When data was provided for both full-burn and end-of-burn periods, both sets of data were analyzed. However, given that temporal resolution of many air quality simulations is on the order of an hour, the 5-minute duration of the end-of-burn data was deemed to be less amenable to implementation. Thus, the results are presented for both cases, but only full-burn data is considered for final determination. Additionally, whenever emissions data were provided from both bivariate and multivariate analysis, both sets of data were considered but finalized determination was based on the multivariate data, given the increased reliability that can be attributed to the observed data. Finally, given the limited detail in the data collected for particulate matter and reported difficulties with sampling and statistical inference from the LBNL experimenters, PM count data were not analyzed.

Consolidated results for the data obtained from cooktop burners are presented in Figure 20 and Figure 21, with the legend for the data presented in Figure 22. Essentially, the boxplot provides measures of the extremes in the sample-based data, from the observed data reported by LBNL. The data points lying along the axis of each boxplot then provide information regarding the sample-based mean and confidence interval as compared to the distribution-based expected and quantile values. As previously mentioned, the expected value is interpreted as the “baseline” emissions change response, while the upper quantile represents the “maximum likely increase,” and the lower quantile represents the “minimum likely increase,” which provide a spanning set of scenarios for implementation in air quality simulations. Additionally, labels above and below each boxplot provide the species name, the selected distribution, and the qualitative and quantitative reliability score. The boxplots for all other data are provided in the Appendix, in Section XXII.A. When both bivariate and multivariate or full-burn and end-of-burn data were available, both sets were analyzed and their boxplots presented. Finally, in the few cases when one outlier was removed, the distribution analysis is provided only for the dataset without the outlier. For example, the NO₂,

END data in Figure 21 had one outlier removed, which can be verified by the difference between the data sample-based mean and the distribution expected value, in spite of the distribution being normal.

In the boxplots, two types of confidence intervals are provided, with a subtle distinction between the two. The confidence interval defined as the “Sample 95% CI” refers to values based on single observed averages. As previously described, the LBNL data provided an average change in emissions per WN change, which represents an average value over multiple experimental tests. The “Sample” confidence interval then refers to the 95% CI around each of these averages, which was data provided by LBNL. The values plotted are then the highest upper confidence limit and lowest lower confidence limit among all sample data points. Thus, the values shown are the most extreme values provided from the LBNL data sets. The “Ensemble 90% CI” is then a confidence interval about the average of all data points in the set (which are themselves averages). Thus, it is the confidence interval around the mean of the attempt to condense the entire data set of averages into the single mean value. This confidence interval is more directly comparable to the 5% and 95% quantiles provided from the distributions since they are formed from the same basis of the entire data set. However, they are not directly comparable given the differences in their definitions. This is apparent as it can be seen that for many distributions determined to be Normal, the “Ensemble 90% CI” and “Distribution Quantile” values are not the same. Although there are exceptions, quantile limits are typically wider than the Ensemble limits, but narrower than the Sample limits.

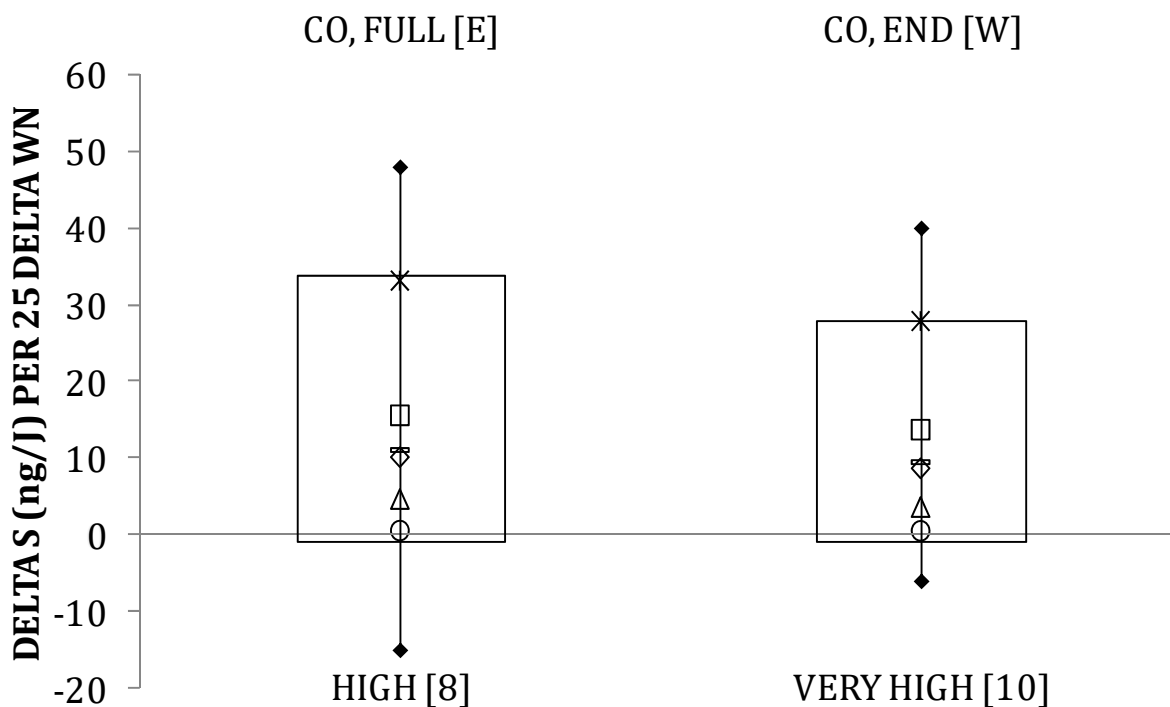


Figure 20: Boxplots for Cooktops, Part 1

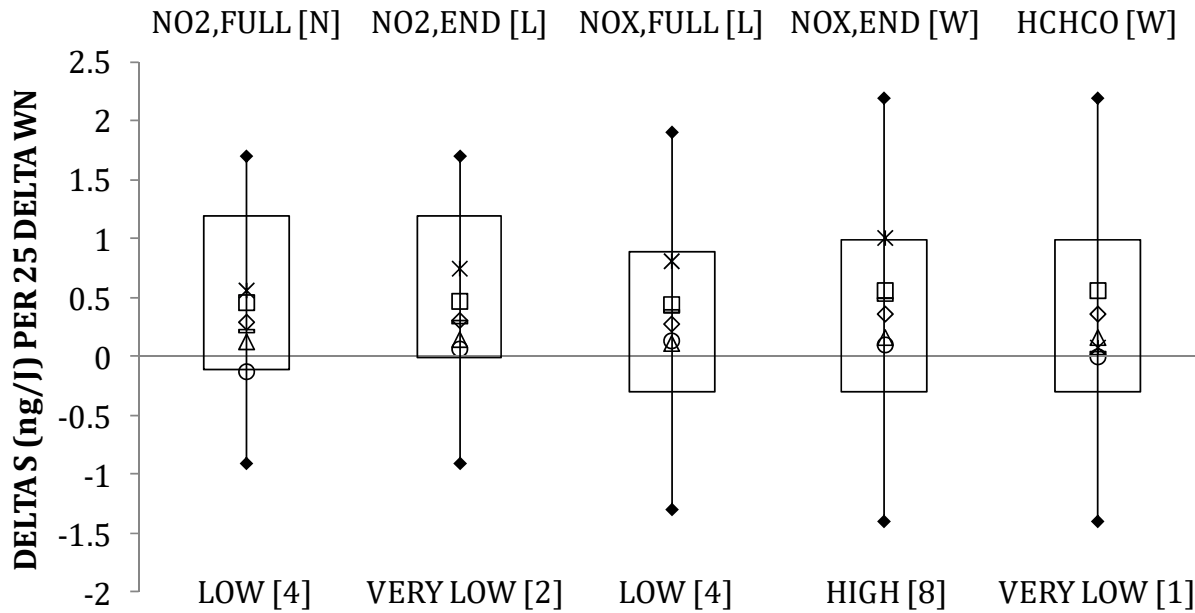


Figure 21: Boxplots for Cooktops, Part 2

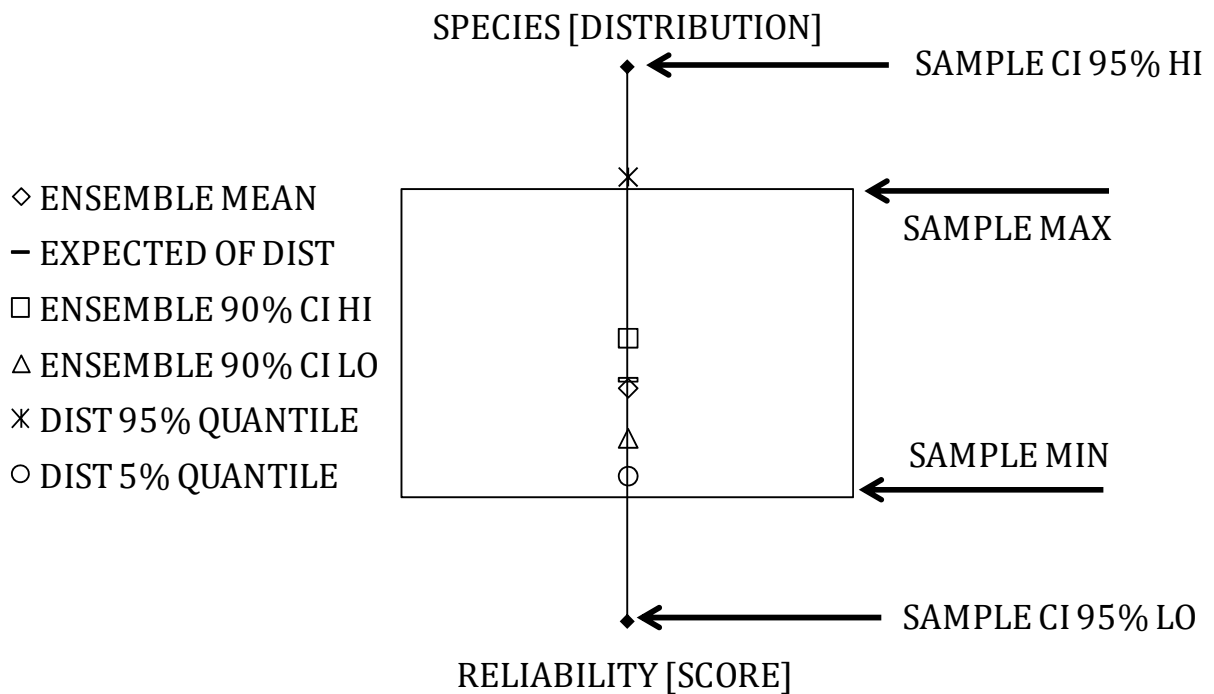


Figure 22: Boxplot Key

From the boxplots, there are a number of important observations that can be made of the sample data that forms the basis of this analysis. For almost all of the data sets, the observed values span

both positive and negative values, and all data sets include Sample confidence intervals spanning positive and negative values. There are even some Ensemble means that are predicted to be negative, while others are predicted to be positive. Thus, it can be expected that similar behavior may be observed in the data derived from the selected distributions. Indeed, such is the case, and it will be seen later that when considering the best engineering estimate and the spanning maximum and minimum likely increases, emission changes with WN may be predicted to be positive or negative. This behavior may be physically justifiable, as there are typically reaction pathways that consume or produce the measured species, which are temperature-dependent. As WN increases, it will typically increase the flame temperature, since the fuel has a higher heat content. However, the burner design can have a supporting or counteracting effect, with the possibility of creating quench zones due to the flame coming into contact with hardware when operated on off-design fuels. With these and other interacting considerations, it is feasible that a range of estimates for the change in emissions respective to WN would include both negative and positive values.

It is also apparent from the boxplots that the magnitudes of the changes in emissions with WN are not equivalent. Typically, changes for CO are the largest (on the order of one to ten), followed by NO₂ and NO_x at one to two orders of magnitude smaller, and finally HCHO, one order smaller than the nitrogen species. Additionally, it can be seen that there was often only a small difference in mean and expected values between full-burn and end-of-burn data, but that the ranges of extreme values in these data sets were often noticeably different. When bivariate and multivariate data were provided, there was a more pronounced difference in mean, expected value, and ranges of extreme values. These observations indicate that care must be taken, and some discernment made between full- vs. end-of-burn and multi- vs. bivariate data sets. As previously stated, this assessment gives preference to full-burn and multivariate data.

Taking all of the boxplots together, it can be seen that by far, the most common distribution selected was the Normal distribution. A summary of the distributions for all data sets is provided in Table 20. For sets where two distributions are provided, the first is the preferred (either multivariate or full-burn) and the second is the less-preferred (bivariate or end-of-burn). When both versions of a data set provided the same result, then the result was reported only once. An asterisk indicates a data set from which a distribution cannot be properly defined due to too few data points (or in one case, 3 data points all at zero). The final, bold column and row provide the most common distribution among all species for a given burner type and all burner types for a given species, respectively. Given these results, it would seem reasonable to typically assume that the most appropriate distribution for any emission factor from any burner type may indeed be best-described by the normal distribution.

Table 20: Distribution Selections for all Data

	CO	NO2	NOx	HCHO	
	<i>E/W</i>	<i>N/L</i>	<i>L/W</i>	<i>W</i>	<i>L/W</i>
Cooktops	N	N/L	N	<i>E/*</i>	N
Broilers	N/L	<i>W/N</i>	N	N	N
Ovens	N	N	N	*	N
Furnaces	N	N	N	*	N
Storage Water Heaters	N	N	<i>L</i>	N	N
Tankless Water Heaters	N	N	N/L	N/*	

Key: N- Normal, L-LogNormal, E-Exponential, G-Gamma
W-Weibull, *- No Distribution

However, there were six distributions for which the final determination was non-normal. As previously mentioned, acceptance of such a determination must come under close scrutiny. Thus, at the conclusion of the mechanistic selection process, these distributions were re-evaluated to simply determine whether or not the non-normal distribution was a clearly preferred distribution. For the CO/Cooktops data, it was found that the Normal distribution was the worst in all three indicator values by a wide margin. NO2/Oven data was similar, with the only exception that the R^2 for the Normal distribution was the second-worst. NOx/Cooktops data could lead to the conclusion that the Normal distribution was a solid second-best distribution, but with indicators sufficiently far from those for the Lognormal that Normal could not be considered equivalent. The Normal distribution's AD was 12% higher, p-value 26% lower, and the R^2 the highest among all distributions. Given the magnitude of the AD and p-value deviations, and that Lognormal had a smaller R^2 deviation from the Normal's value, the Lognormal determination seems reasonable. NOx/Tankless Water Heaters had the same characteristics as CO/Cooktops. The Weibull determination for HCHO/Cooktops is also reasonable determination, given that the Normal was the worst in AD and p-value, but had the highest R^2 . Finally, the HCHO/Broilers was the only distribution that could possibly be adjusted to Normal. In this case, Normal had the best AD, was off by 30% in p-value, and 2% off in R^2 .

Thus, for all but the HCHO/Broilers, the indicated non-normal distributions seem like they should remain as determined. However, even the HCHO/Broiler data may indeed remain as exponential. After removal of non-negative data, this determination was made based on exceedingly few data points (only three). Moreover, the expected values for the Normal and Exponential distributions are exactly the same. Only the quantile values differ, and it is by a small amount. Thus, all non-normal distributions may stand as determined. It is interesting to note that half of these occurred in data sets related to cooktops. This was the most robust data provided by LBNL, with the largest original sample size and typically the least number of non-positive data. Thus, in these data sets, the non-normal distributions suffered a particularly small disadvantage in the R^2 determination due to loss of data points. This can be seen by comparison of the multiple histograms (with overlaying distribution functions) and cumulative probability distribution functions provided in Sections XXII.C and XXII.D, respectively. Therefore, there does exist the possibility that at least some of the other distributions identified as normal may have a somewhat biased determination due to the small amount of positive data in these sets.

The detailed results are not shown in this work, but as an alternative, the distribution selection process was repeated with the adjustment of basing R^2 for non-Normal distributions on histograms

and empirical cumulative distribution functions derived from only the positive data in each set. Importantly, this adjustment removes one of the previously-discussed biases towards the Normal distribution. Thus, the results of such an analysis must be considered carefully and may not be as reliable as the results already presented. When the distributions were analyzed in this manner, the determinations were as shown in Table 21. It is immediately noticeable that the Normal distribution becomes much less common and the variability in the identified distributions is much greater compared to the previous method. Additionally, for the most part, the non-Normal distributions from Table 20 are replicated in this method. This suggests the possibility that increased volumes of data will result in more determinations of non-Normal distributions. However, given the caveat already discussed and the fact that the determinations in Table 21 are based on exceptionally small data sets, such a determination cannot be made with certainty from the observed data utilized in this work.

Table 21: Distribution Selections for Adjusted R² Method

	CO	NO2	NOx	HCHO	
Cooktops	E	N/E	L	E	E
Broilers	*G/N	*G	*G	E/*	G/*
Ovens	N/L	G/W	N	L/*	N/L
Furnaces	N/L	N/*	N	*	N/L
Storage Water Heaters	L/*	G/*	L	*	L
Tankless Water Heaters	L/*	E	L	N	L
	L/*	G/*	L/N	E/*	

Given these considerations, the final determination of the three desired emission factor increases was based on the distributions shown in Table 20. There were only two exceptions, both of which were related to the HCHO data. As shown in the table, HCHO/Furnaces and HCHO/Storage Water Heaters were not represented by any distribution. This was due to the nature of the observed data provided. For the furnaces case, only three data points were provided, and their values were evenly spaced. Thus, the median was chosen as the best engineering estimate while the maximum and minimum values were utilized as the maximum and minimum likely increase. For the storage water heater data, there were again only three data points provided. However, they were all zero. Thus, all estimates are simply set to zero for this case as well. This was observable in the related boxplot for HCHO/Storage Water Heaters. All emission factor increase estimates are provided in Table 22.

From Table 22, it can be seen that although it was previously suggested that a single distribution shape could likely be utilized for most of the data (and thus by extension, most data for a given emissions species or burner with the other classification varying), a single numeric value cannot be used for the estimate of emissions change. For example, considering only the best engineering estimate, the emissions of CO across all burner types not only spans a wide range of orders of magnitude but also includes both positive and negative predictions. Likewise, the previously-noted differences in orders of magnitude across species does not allow for a single estimate to be used for the same burner type across various species. Thus, although the most idealized data would be able

to provide a single estimate for a given species across all burners, this work finds that such a simplification cannot be made. The numerous differences in burner design and operation provide too many physical differences to confidently state that emissions change with respect to WN is independent of burner design. Moreover, for the same burner, the emissions change with respect to WN is not independent of the measured species.

Table 22: Emission Increase Estimates for Three Spanning Scenarios (ng/J per 25 WN)

	Best Engineering Estimate	Maximum Likely Increase	Minimum Likely Increase
	<u>CO</u>		
Cooktops	11.0833	33.2027	0.5685
Broilers	6.1667	17.0484	-4.7151
Ovens	12.5455	26.0164	-0.9255
Furnaces	-0.7500	1.6285	-3.1285
Storage Water Heaters	0.1867	0.9859	-0.6126
Tankless Water Heaters	3.9400	19.0676	-11.1876
	<u>NO2</u>		
Cooktops	0.3667	0.9278	0.0397
Broilers	0.1167	0.8021	-0.5688
Ovens	0.4132	0.9857	0.0557
Furnaces	-0.0500	0.1767	-0.2767
Storage Water Heaters	0.0017	0.2557	-0.2524
Tankless Water Heaters	0.2300	0.6448	-0.1848
	<u>NOx</u>		
Cooktops	0.3928	0.8179	0.1422
Broilers	0.3333	1.5361	-0.8694
Ovens	-0.1833	0.5033	-0.8699
Furnaces	0.6000	1.5263	-0.3263
Storage Water Heaters	0.1167	0.6307	-0.3974
Tankless Water Heaters	1.7383	5.2478	0.2376
	<u>HCHO</u>		
Cooktops	0.0383	0.0850	0.0067
Broilers	0.0433	0.1298	0.0022
Ovens	-0.0036	0.0606	-0.0679
Furnaces	-0.0400	-0.0200	-0.0600
Storage Water Heaters	0.0000	0.0000	0.0000
Tankless Water Heaters	-0.0500	0.0502	-0.1502

Finally, the results presented in Table 22 must be considered in light of their associated reliability estimates. The breakdowns of these estimates are provided in Section XXII.E. Table 23 provides a summary of all emission factor reliability estimates, consolidated from the individual boxplots. The range of reliabilities for all estimates varied widely. It is interesting to note that the HCHO data had the lowest scores in reliability on average, and this was the data that had the smallest magnitude.

Additionally, the sample-based reliability for HCHO were typically very low; this seems to indicate the observed data itself, with such small orders of magnitude, may have had some difficulty with resolution and sensitivity, leading to the low reliability and difficulty in finding an appropriate distribution. Also, the range of values for a given emission factor, relative to the best engineering estimate, did not seem to be correlated to the reliability score. For most emissions factors, the range of values was between 1 and 10 times the best estimate. The largest ratio did not always occur at the lowest reliability scores, though. For example, both CO/Ovens and HCHO/Cooktops had relative ranges near 2. However, their reliability ratings were 8 and 1, respectively.

Additionally, the reliability was not correlated to the type of distribution selected. Comparison of Table 20 and Table 23 reveals that the data sets identified as Normal acquired reliability ratings at nearly every possible value. A similar observation can be made for the data sets that were found to be non-normal (though the limited amount of such data limits the interpretation). Finally, the sample size of a data set was also not a good indicator of the reliability when considered alone. Given that the reliability score was defined with a large number of desirable features of the observed data sets and the selected distribution to represent the set, these observations are not entirely surprising. The reliability score developed is thus determined to be a fairly robust indicator of the confidence that a researcher may have in implementing the identified emission factors.

Table 23: Summary Emission Factor Reliability Scores

	CO	NO2	NOx	HCHO
Cooktops	8/10	4/2	4/8	1
Broilers	8/5	7	4	6
Ovens	8	10/8	9	3
Furnaces	10/5	1	7	3
Storage Water Heaters	4	9	2	*
Tankless Water Heaters	4	5	7	6

Finally, it is important to consider these projected increases in emissions relative to WN as they compare to typical emission rates within the area of interest. The minimum and maximum best engineering estimates for each emission species were utilized in this work as points of comparison. Typical emission rates and natural gas consumption rates within the Southern California Air Basin were estimated as in previous work [10]. For the comparison, the heating value of natural gas was assumed to be 1000 BTU per standard cubic foot and the WN was assumed to be 1335 BTU per standard cubic foot, per the prior work. Table 24 provides the results of this comparison. It can be seen that the minimum values of the expected daily increase are typical one or two orders of magnitude below the typical daily emission, calculated on a heat content and WN specific basis. However, the largest emissions estimates within each set approach parity with the typical emission value or one order of magnitude below. Thus, it is expected that the emissions changes estimates provided in this work will, for some burner types and species, provide a significant increase to the emissions predicted for a given WN scenario (given the experimental limits, WN can increase by 85 units with the predicted values; thus, just over three times the presented rates (85/25) may be

implemented in extreme cases). However, some increases are likely negligible and at the time of implementation of the simulation may likely be ignored. This determination will be most appropriately considered by the researcher performing the simulation.

Table 24: Comparison of Typical Daily Emission Rates and Projected Increases for the South Coast Air Basin in Southern California

	Typical Emission (tons/day)	Energy-Specific Emissions (ng/J)	Energy-and-WN- Specific Emissions (ng/J/25WN)	Emissions Factor Increase Range (ng/J/25WN)
CO	2358.42	827.95	15.50	[-0.75, 12.545]
NO2	21.69	7.62	1.43	[-0.05, 0.413]
NOx	216.92	76.15	0.14	[-0.183, 1.738]
HCHO	15.70	5.51	0.10	[-0.050, 0.043]

XX Conclusions

This work has developed a method of estimating emission factor changes with respect to fuel WN for residential burners. The method was developed on the basis of assuming that the data sets available to a researcher interested in these metrics are too small to perform rigorous statistical inference. Thus, the method developed in this work seeks to provide conservative estimates of the distribution shape that may give rise to the observed data, and provide a more accurate estimate of the best engineering guess and possible extreme values of the emissions change rates. Due to these assumptions, the method gives preference to the Normal distribution when possible, since it is expected that this distribution is the most likely to properly describe the majority of the data in the application and any conclusions pointing to other distributions must be made with careful consideration of likelihood and ample supporting indicators. Additionally, the method provides context to the estimates that are developed by providing a way to assess the reliability of a given estimate, based on desirable features of both the observed data set as well as the selected distribution shape. The method is generalized and can therefore be utilized by researchers attempting to develop these types of estimates for any set of burner types, emissions species, and fuel WN that are important to a given area, provided the researcher has access to proper, representative data.

This work additionally applied this method to data provided by an LBNL study regarding the emissions changes based on WN for residential burners. The analysis found that for most combinations of burner type and emissions species, the Normal distribution should be considered the most-representative distribution for the data. However, for cases when the Normal distribution was not found to be a good representative, it was clear that this distribution should not take the place of the distribution identified by the mechanistic method described. Additionally, extreme values of predicted emissions changes are taken not from confidence intervals around the mean, but from 5% and 95% quantiles, as the latter can be calculated from any distribution shape, but not

the confidence interval about the mean (without advanced techniques that may involve too much extrapolation from limited data). It was also additionally determined that the reliability measure developed as part of the distribution selection method was robust, due to its inclusion of multiple desirable features of the observed data and selected distribution in its calculation. Considering single parameters as indicators did not match well to the calculated reliability.

Thus, the emission change estimates predicted by this work may be utilized in future investigations of regional air quality impacts due to natural gas interchangeability. Alternatively, the analysis method described could be applied to other data sets that may be more complete or offer desirable features that the example set did not. Both of these options can provide informative bases for future regional air quality impact investigations.

XXI References

- [1] Natural Gas Council: Gas Interchangeability Work Group. White Paper on Natural Gas Interchangeability and Non-Combustion End Use. 2005.
- [2] Williams, T. 2006. Staff Paper: Technical Background and Issues of Gas Interchangeability, Arlington, American Gas Association.
- [3] United States Environmental Protection Agency. ENERGY STAR Program Requirements, Product Specification for Furnaces, Eligibility Criteria, Version 3.0: Draft. Washington, DC, 2010.
- [4] American Gas Association and Gas Appliance Manufacturers Association: American Gas Association Laboratories. Fundamentals of Gas Combustion, Revised. 1996.
- [5] Williams, T. 2005. Assessment of Changes to the Performance of Gas Appliances in Relation to Variations in Gas Quality, London, Department of Trade and Industry.
- [6] Bourns College of Engineering: University of California, Riverside. Final LNG Research Study White Paper Version 2.0. 2004.
- [7] Kirk, W.B .and Griffiths, J.C. 1958. Applying Fundamental Concepts to the Engineering Design of Appliance Burners, Cleveland, American Gas Association Laboratories.
- [8] Johnson, F. and Rue, D.M. 2003. Gas Interchangeability Tests: Evaluating the Range of Interchangeability of Vaporized LNG and Natural Gas, Final Report, Des Plaines, Gas Technology Institute.
- [9] Singer, B.C., et al. Natural Gas Variability in California: Environmental Impacts and Device Performance: Experimental Evaluation of Pollutant Emissions from Residential Appliances. LBNL-XXXX, 2009.
- [10] Carerras-Sospedra, M., et al. Air Quality Impacts of Liquefied Natural Gas in the South Coast Air Basin of California. California Energy Commission. Publication Number: CEC-500-2011-041. 2011.

XXII Appendix

XXII.A Emission Factor Boxplots

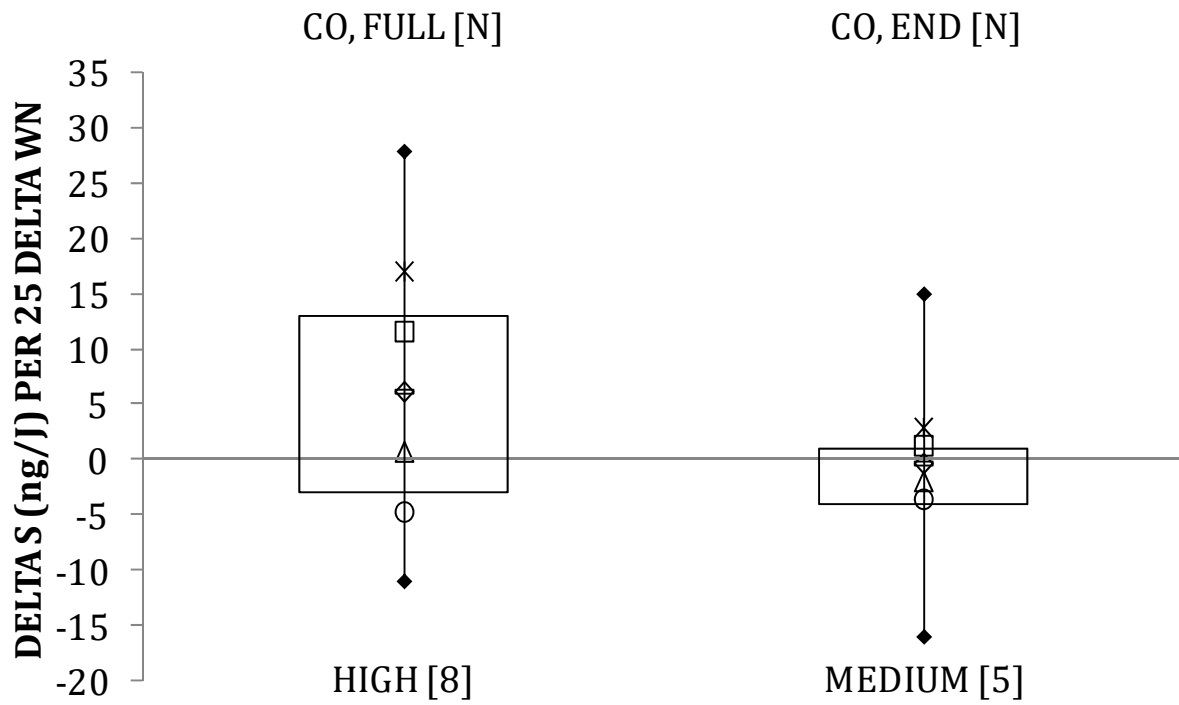


Figure 23: Boxplots for Broilers, Part 1

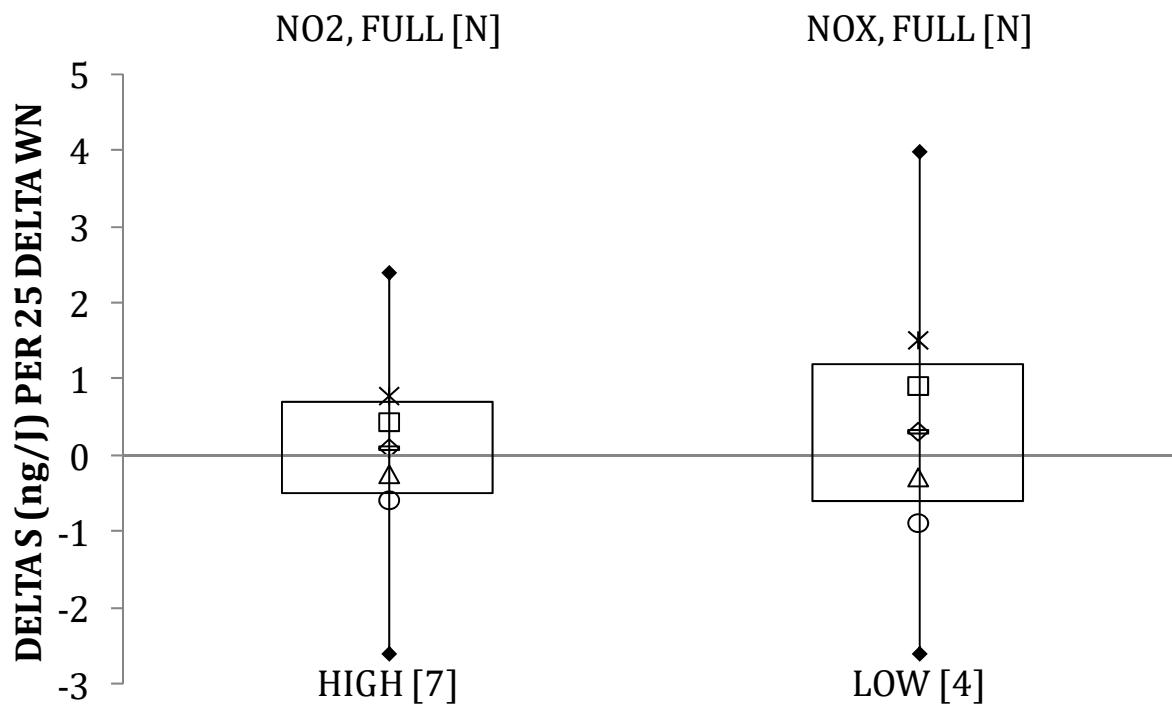


Figure 24: Boxplots for Broilers, Part 2

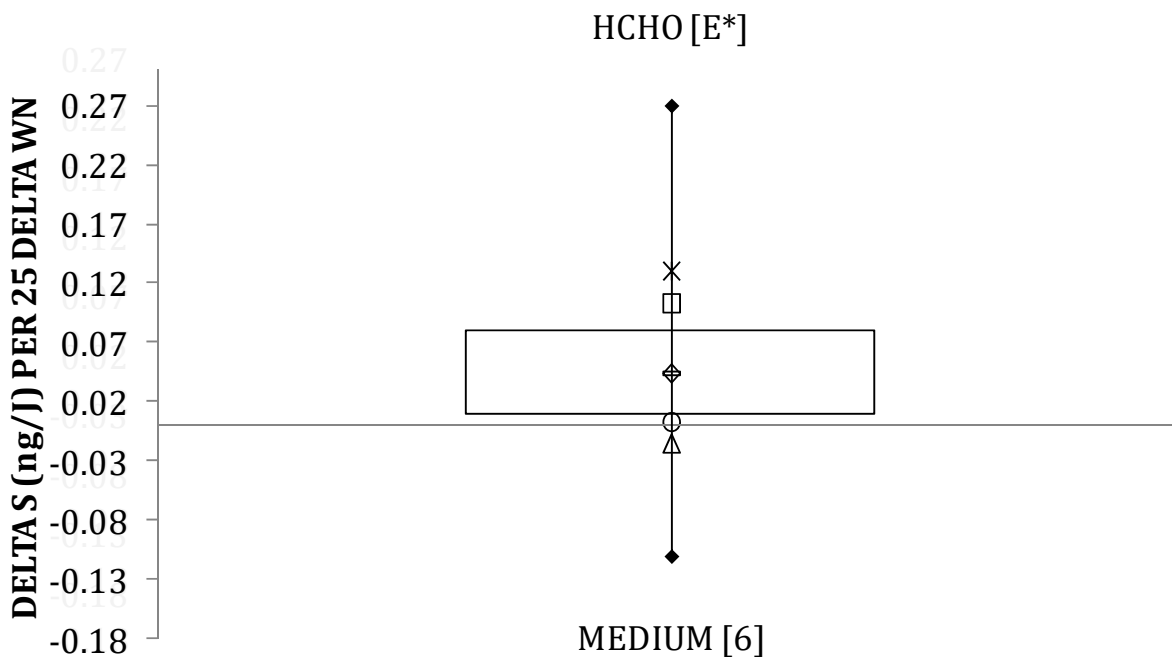


Figure 25: Boxplots for Broilers, Part 3

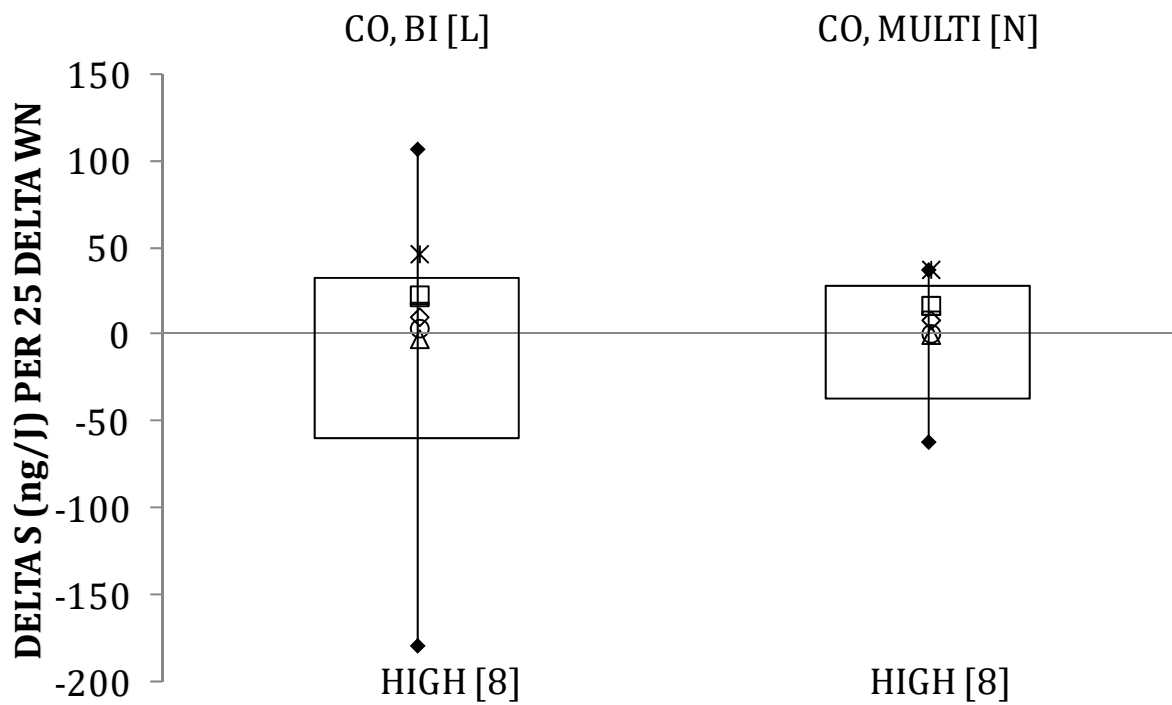


Figure 26: Boxplots for Ovens, Part 1

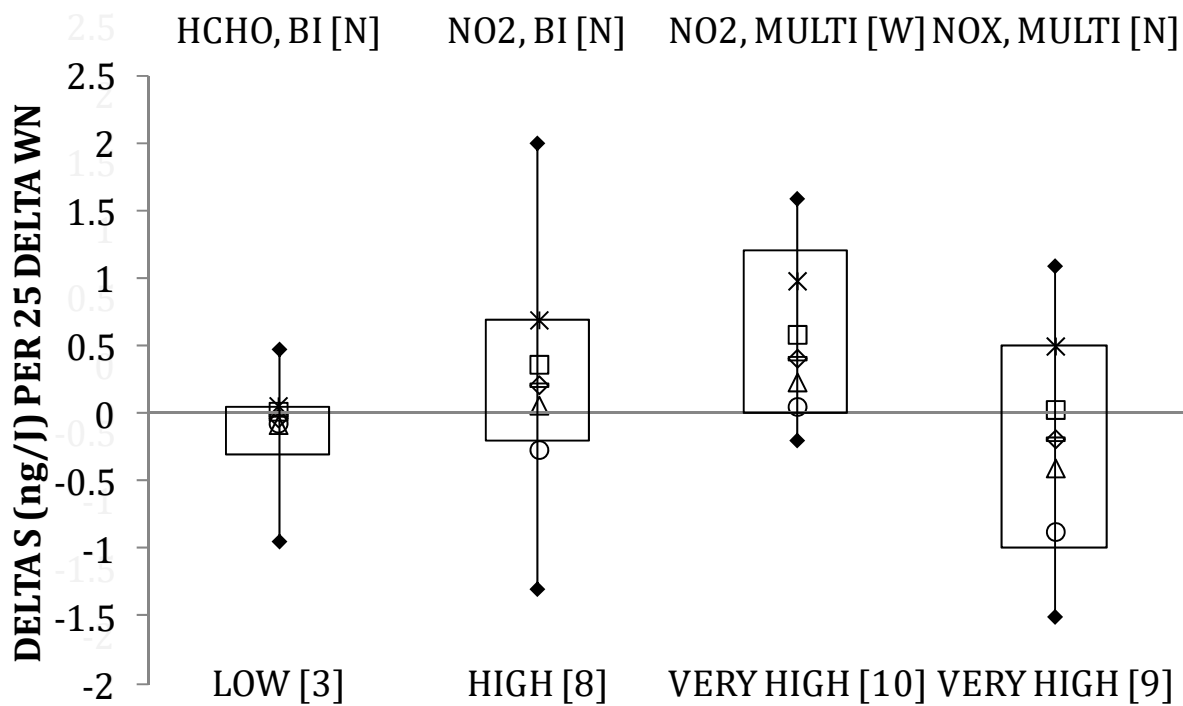


Figure 27: Boxplots for Ovens, Part 2

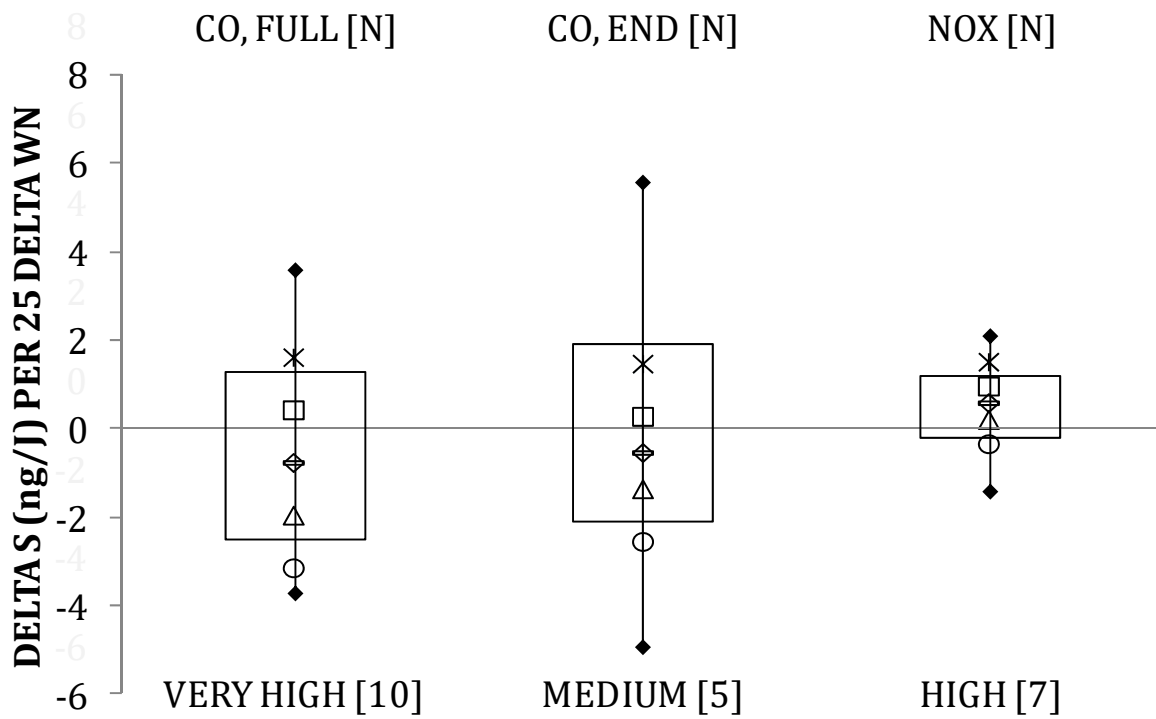


Figure 28: Boxplots for Furnaces, Part 1

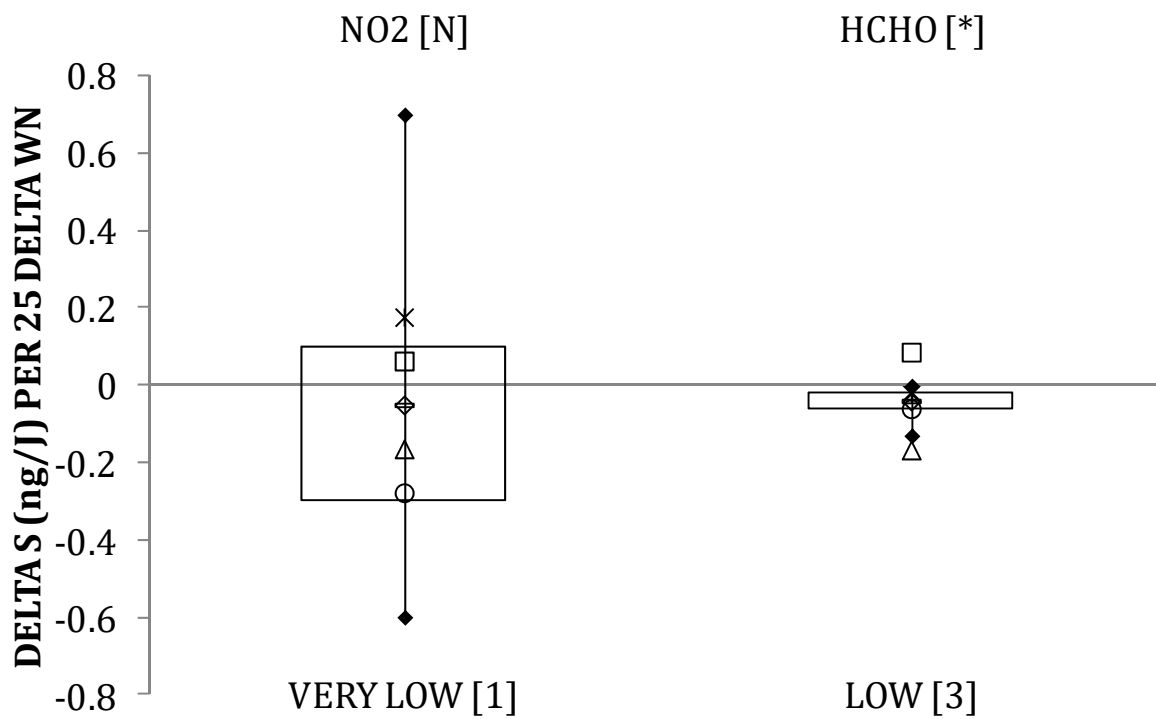


Figure 29: Boxplots for Furnaces, Part 2

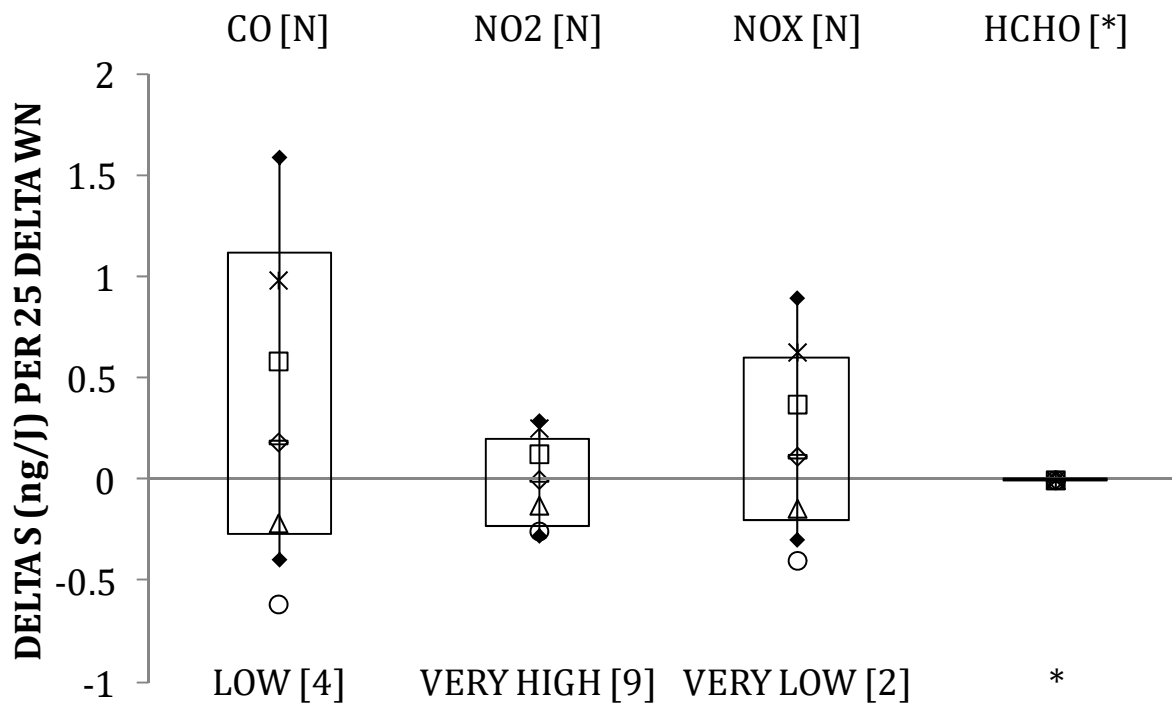


Figure 30: Boxplots for Storage Water Heaters

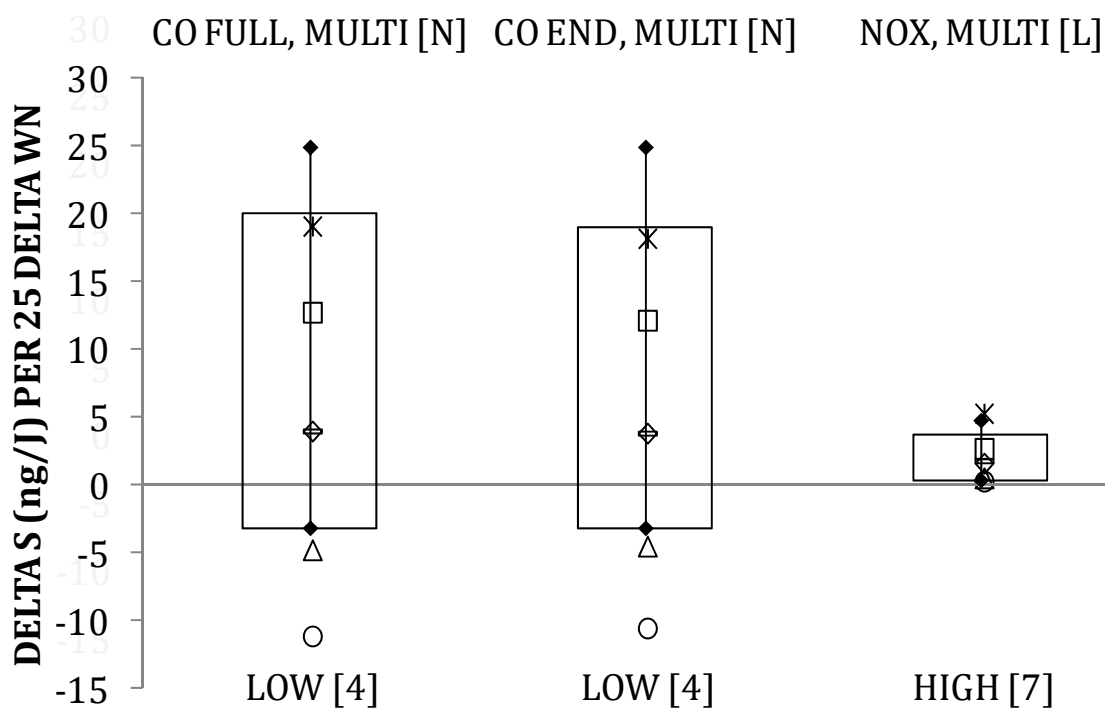


Figure 31: Boxplots for Tankless Water Heaters, Part 1

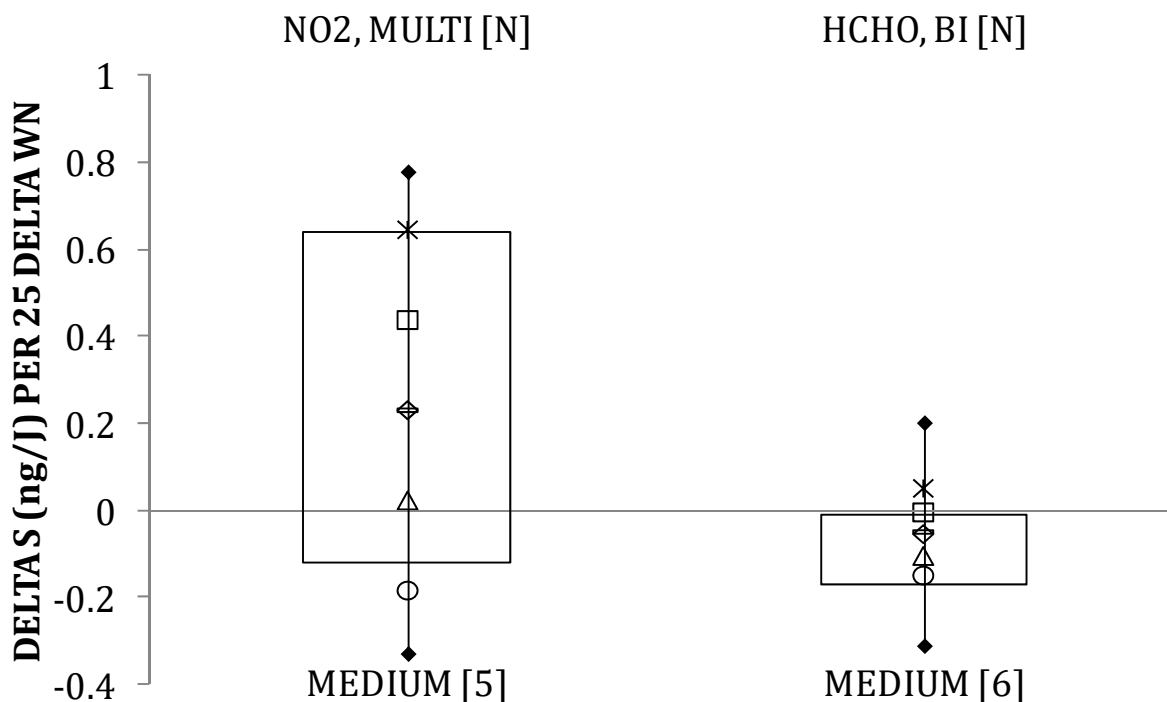


Figure 32: Boxplots for Tankless Water Heaters, Part 2

XXII.B Distribution Selection Tables

In the following tables, bold distributions in the R^2 column indicate those distributions for which this indicator in the most favorable distribution was at least 10% higher than the second-most-favorable distribution. Distribution initials are as previously described in Table 20 with the addition of k, which indicates a Gamma distribution with shape parameter approximately equal to 1, thereby resulting in a distribution equivalent to the Exponential distribution.

Table 25: Distribution Selection Table, Cooktops

	AD	p-val	R2	Determination	2nd Round	Determination2	BestAverage	Determination 3
CO, Full	W	k,W	L		L,k,W		E	E
CO, End	k	k,W	W	W			E	
NO2 Full, No Outlier	N	N	W		N	N	N	
NO2 End, No Outlier	L	E	W				L	L
HCHO, No Outlier	W	E	N				W	W
NOX, Full	L	L	N		L	L	L	
NOX, End	G	L,G,W	N		L,G,W	W	L	

Table 26: Distribution Selection Table, Broilers

	AD	p-val	R2	Determination	2nd Round	Determination2	BestAverage	Determination 3
CO, Full	N	N,G,W	N	N			N	
CO, End	N	N	N	N			N	
NO2, Full	N	N,G,W	N	N			N	
HCHO	N	E,G,W	E	E			E	
NOX, Full	L	L,G,W	N				N	N

Table 27: Distribution Selection Table, Ovens

	AD	p-val	R2	Determination	2nd Round	Determination2	BestAverage	Determination 3
CO, Bi	L	L,G	L	L			L	
NO2, Bi	W	N,G,W	N	N			N	
HCHO, Bi	L	G	N				N	N
CO, Multi	N	E	N	N			N	
NO2, Multi	L	L,G,W	W	W			L	
NOX, Multi	L	N,G,W	N	N			N	

Table 28: Distribution Selection Table, Furnaces

	AD	p-val	R2	Determination	2nd Round	Determination2	BestAverage	Determination 3
CO, Full	N	N,k	N	N			N	
CO, End	N	N	N	N			N	
NO2, Full	E	E	N				N	N
NOX	N	N	N	N			N	

Table 29: Distribution Selection Table, Storage Water Heaters

	AD	p-val	R2	Determination	2nd Round	Determination2	BestAverage	Determination 3
CO	L	k,W	N				N	N
NO2	N	N,G,W	N	N			N	
NOX	L	G,W	N				N	N

Table 30: Distribution Selection Table, Tankless Water Heaters

	AD	p-val	R2	Determination	2nd Round	Determination2	BestAverage	Determination 3
HCHO, Bi	N	N	N	N			N	
CO Full, Multi No Outlier	L	L,G,W	N				N	N
CO End, Multi No Outlier	L	E	N				N	N
NO2 Multi	L	L,G,W	N				N	N
NOX, Multi	L	L,G,W	E		L,E		L	L

XXII.C Distribution Histograms

Horizontal axes in the following figures are all changes in emission rates (ng/J) per change of 25 in WN. Vertical axes are counts of data points at the corresponding emission change rate or within the corresponding bin for distribution trends and the histogram, respectively.

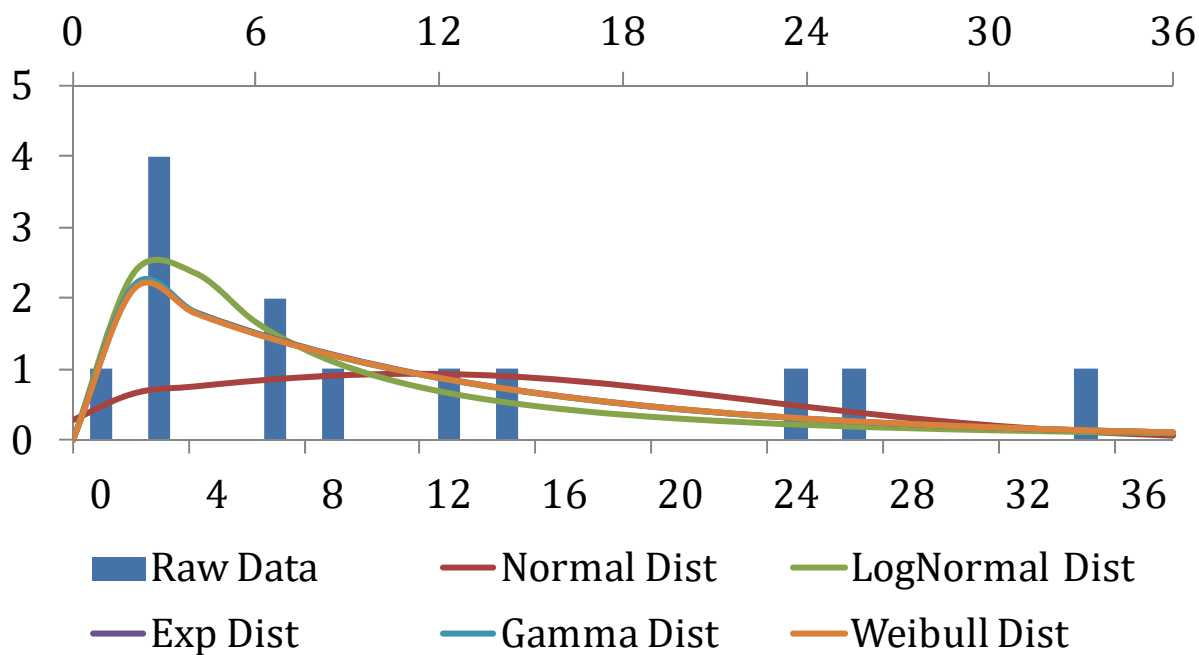


Figure 33: Histogram, CO, Full/Cooktops

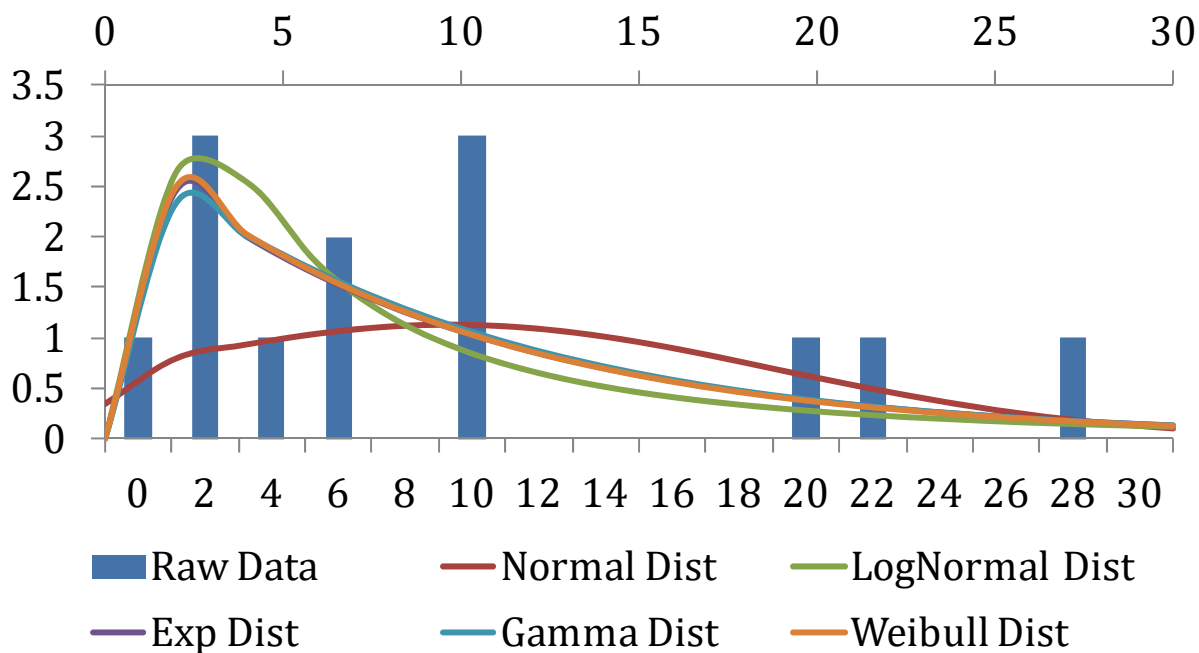


Figure 34: Histogram, CO, End/Cooktops

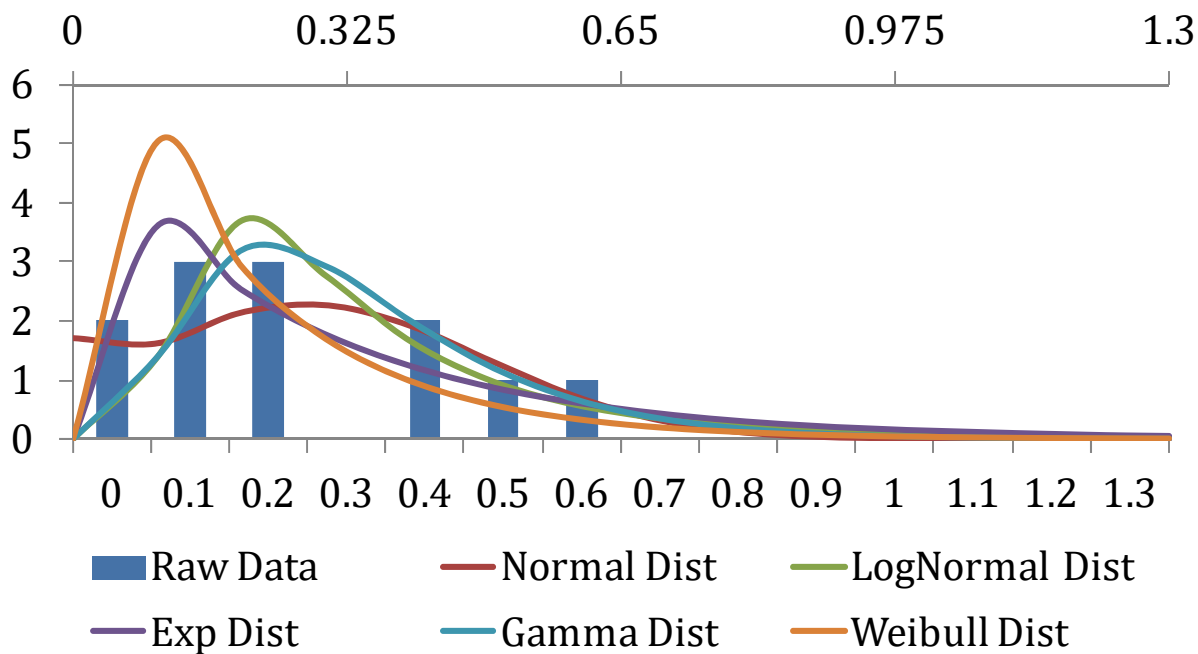


Figure 35: Histogram, NO2, Full/Cooktops

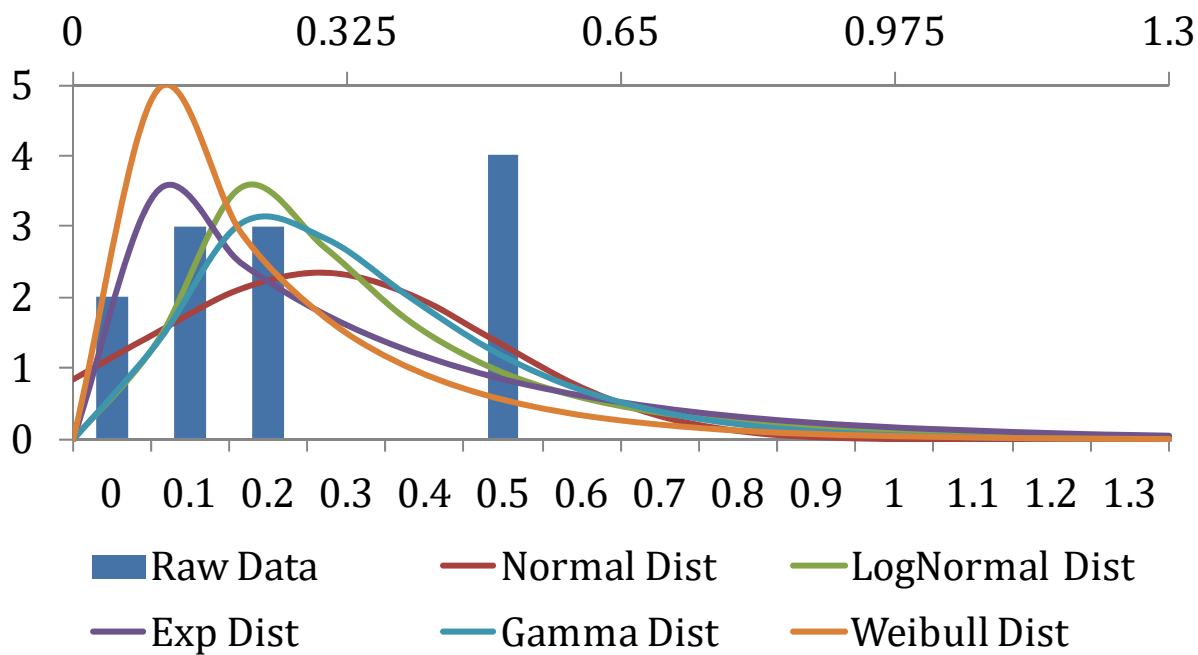


Figure 36: Histogram, NO2, End/Cooktops

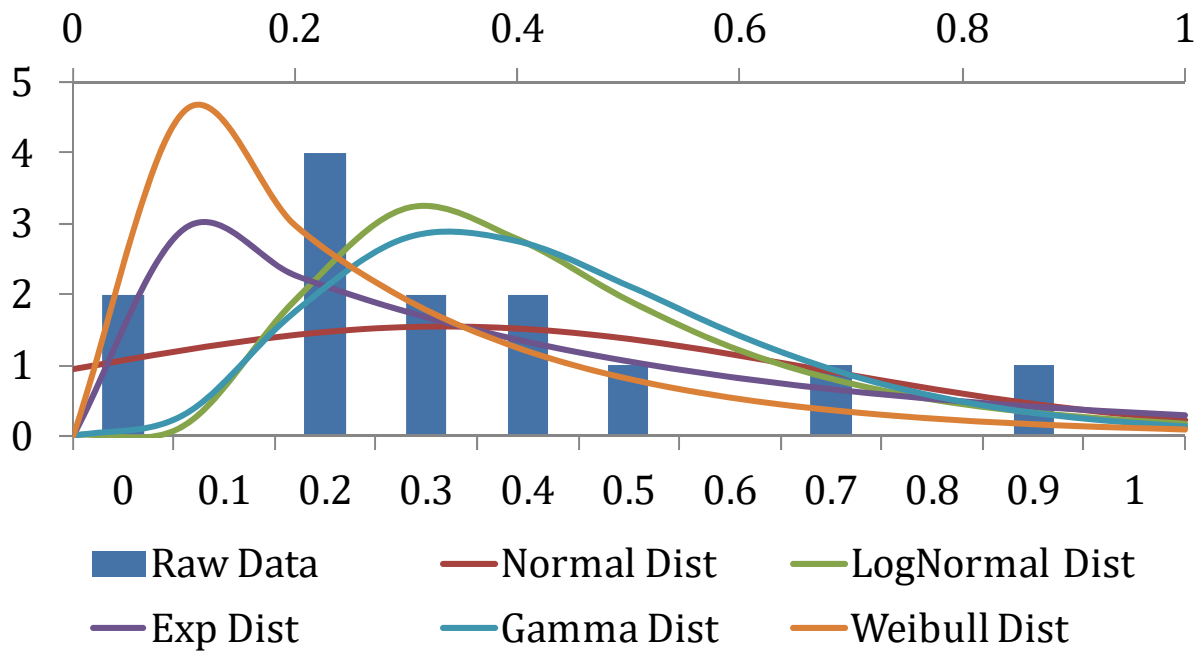


Figure 37: Histogram, NOx, Full/Cooktops

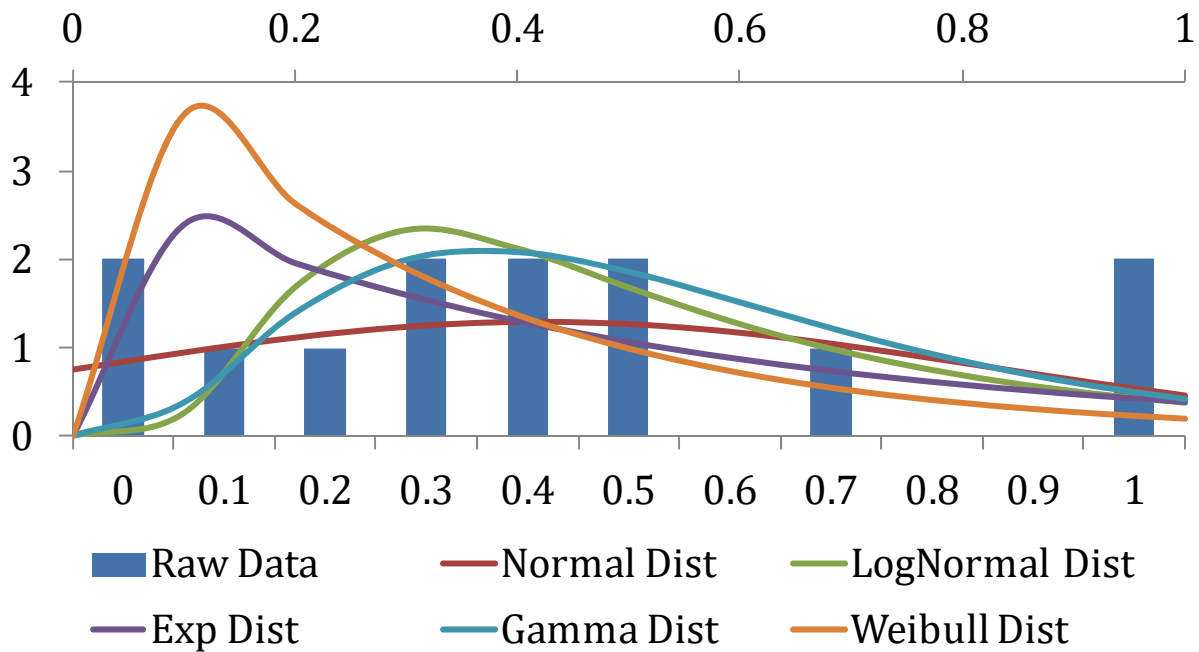


Figure 38: Histogram, NOx, End/Cooktops

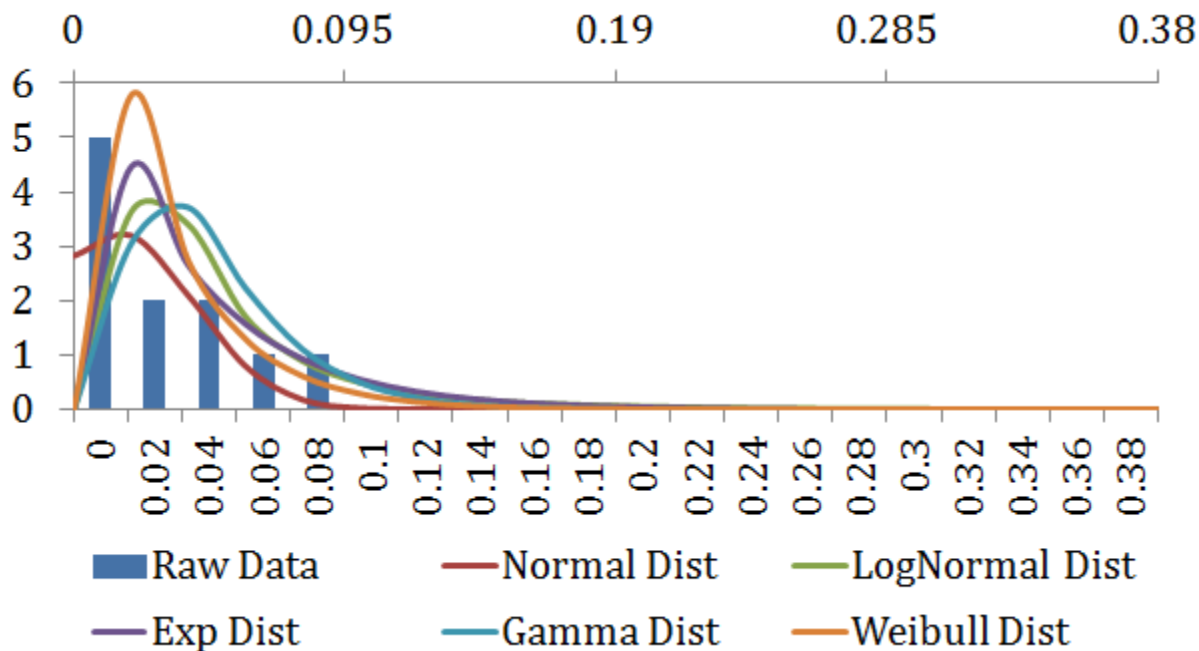


Figure 39: Histogram, HCHO/Cooktops

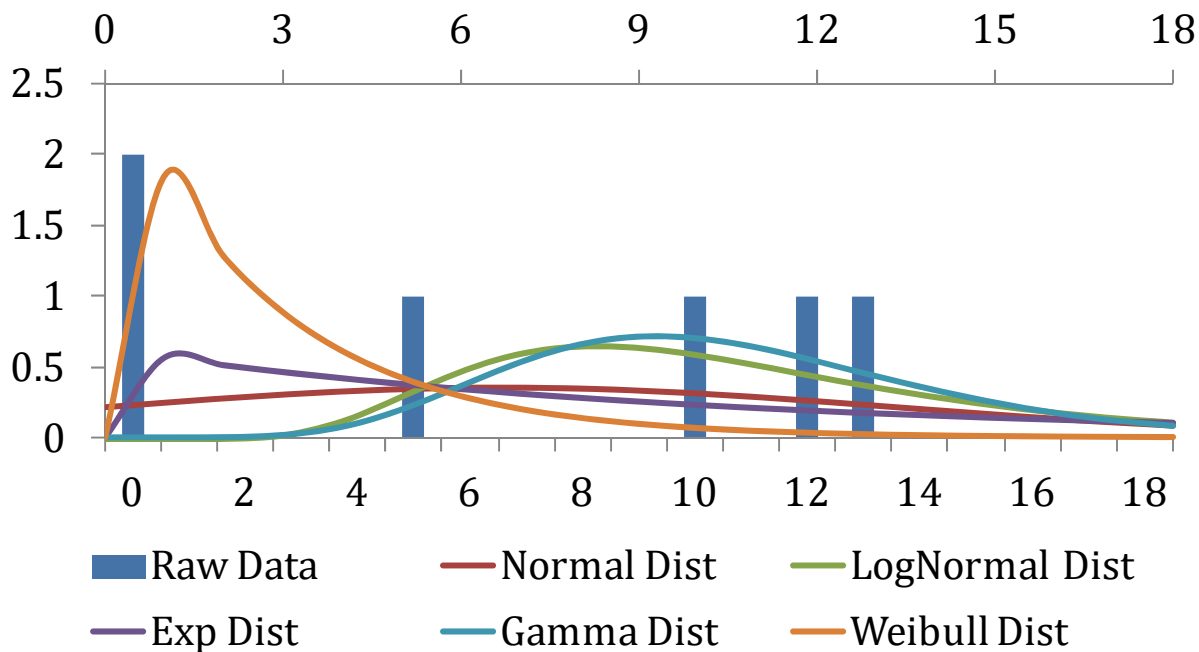


Figure 40: Histogram, CO, Full/Broilers

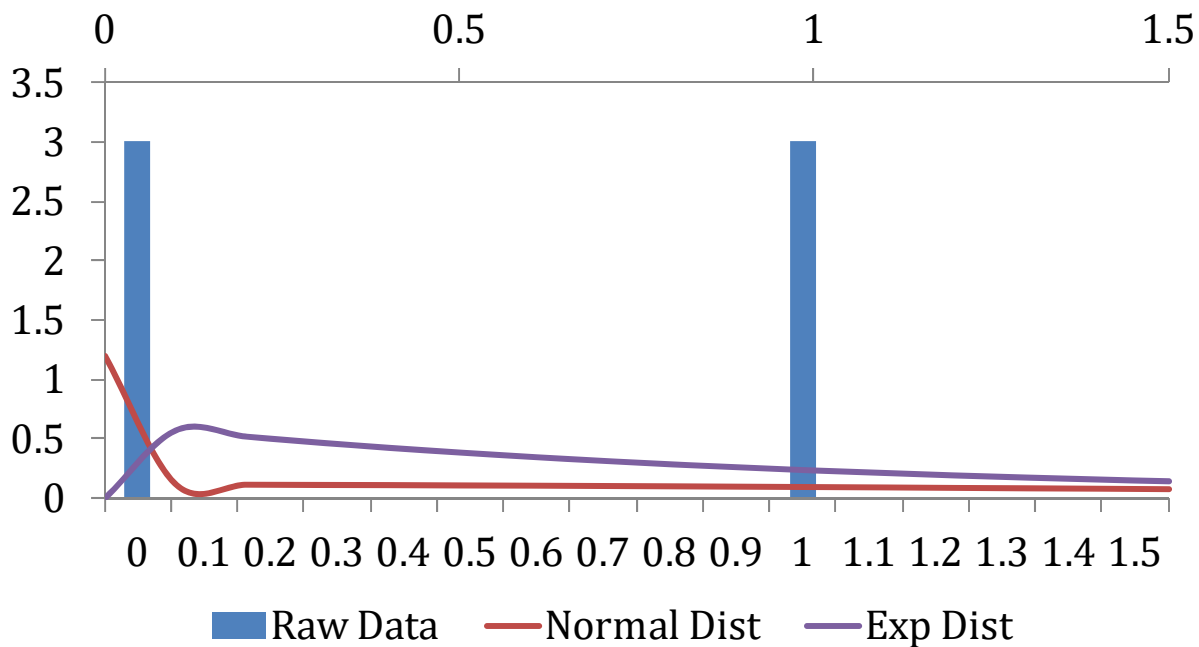


Figure 41: Histogram, CO, End/Broilers

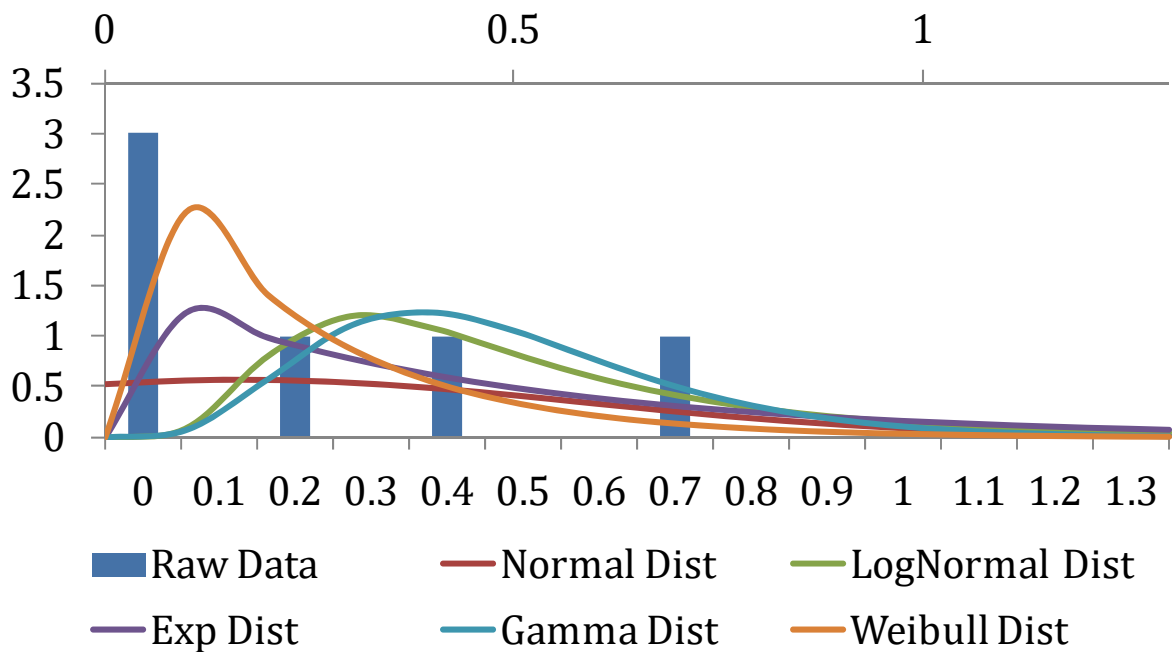


Figure 42: Histogram, N02/Broilers

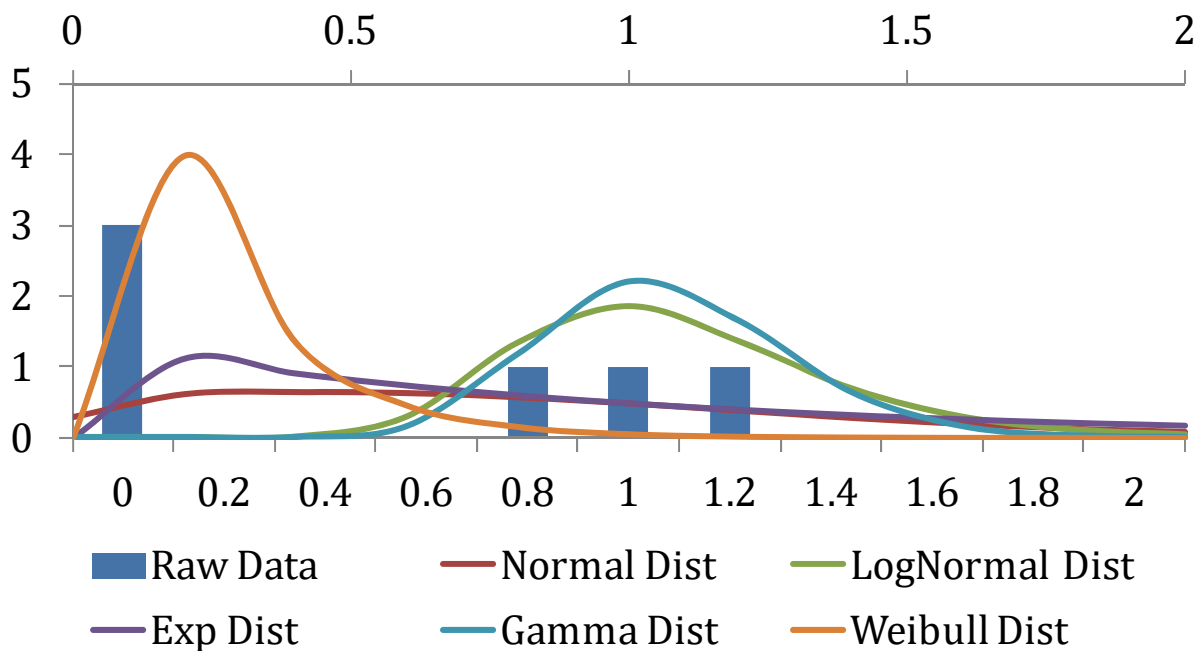


Figure 43: Histogram, NOx/Broilers

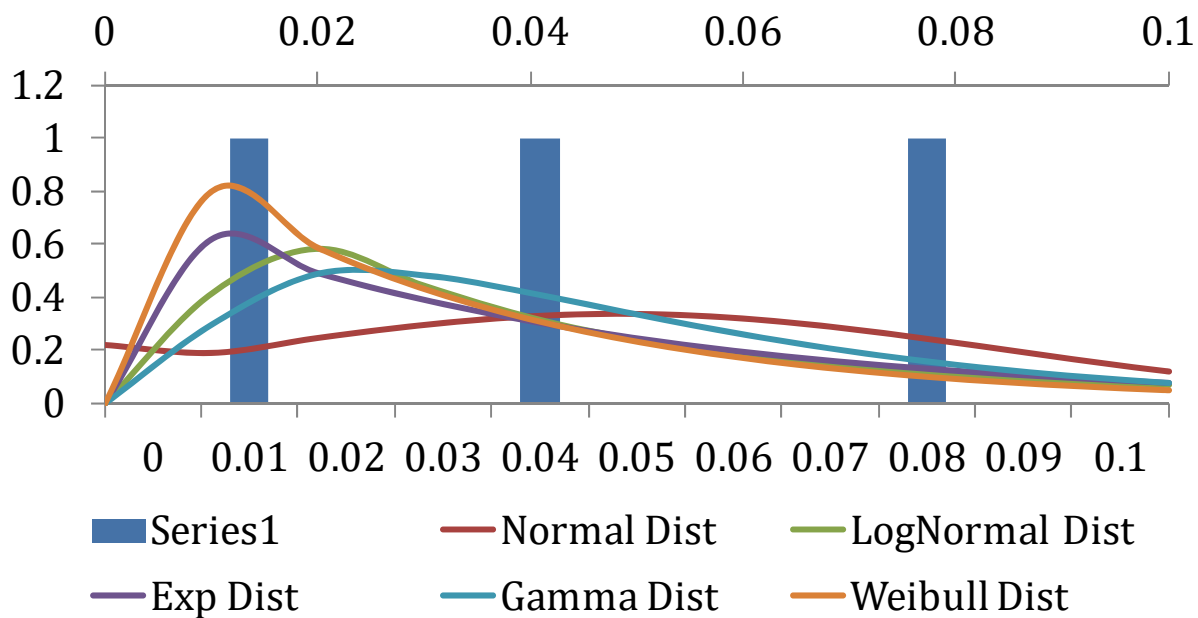


Figure 44: Histogram, HCHO/Broilers

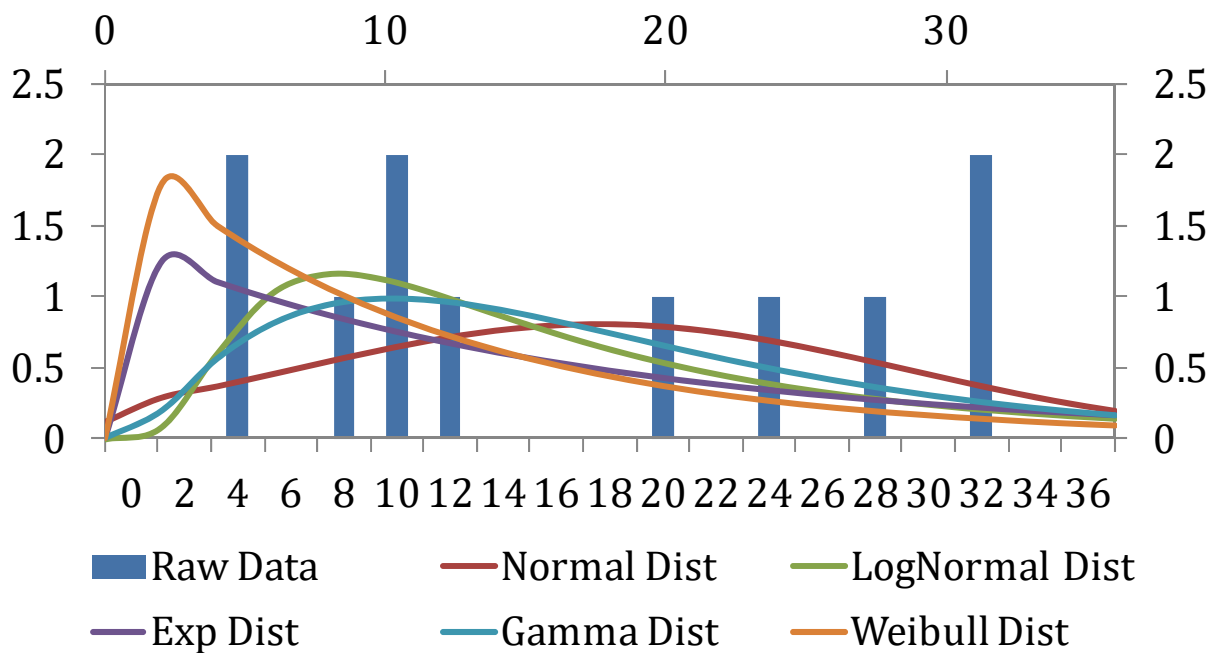


Figure 45: Histogram, CO, Bivariate/Ovens

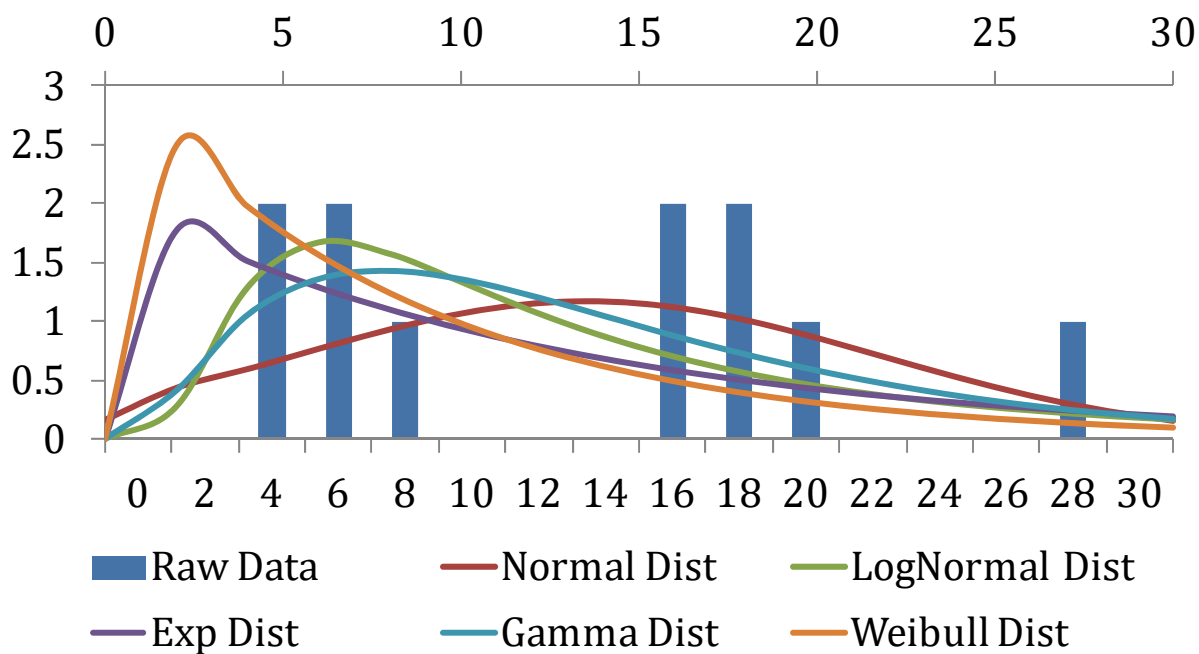


Figure 46: Histogram, CO, Multivariate/Ovens

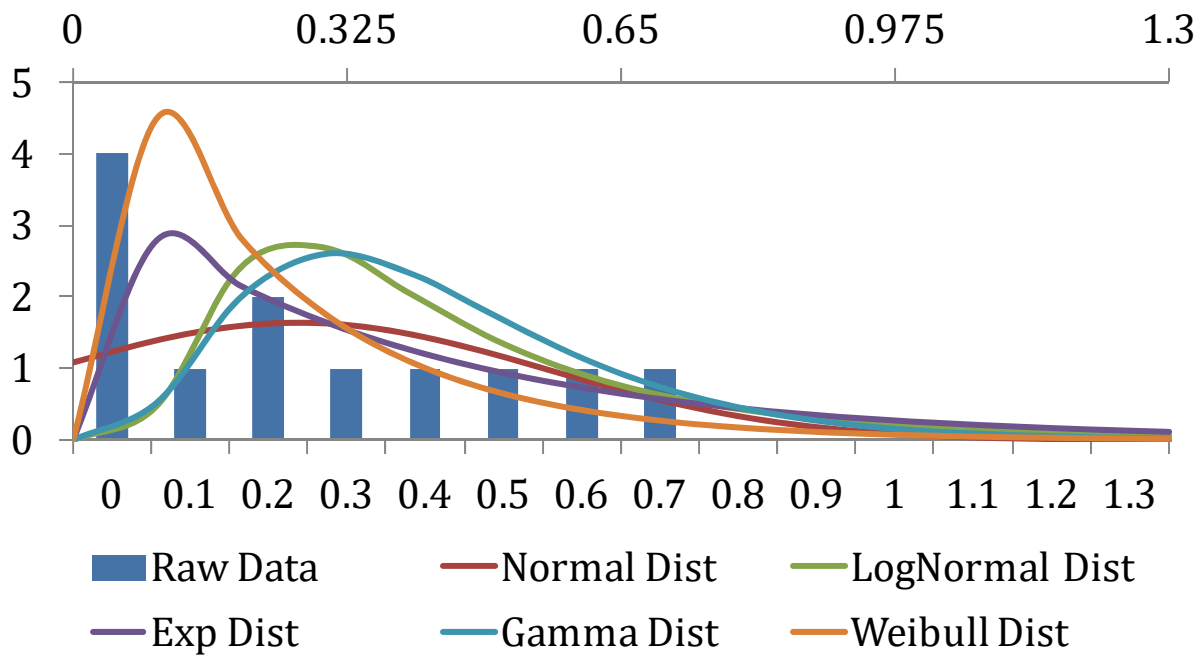


Figure 47: Histogram, NO2, Bivariate/Ovens

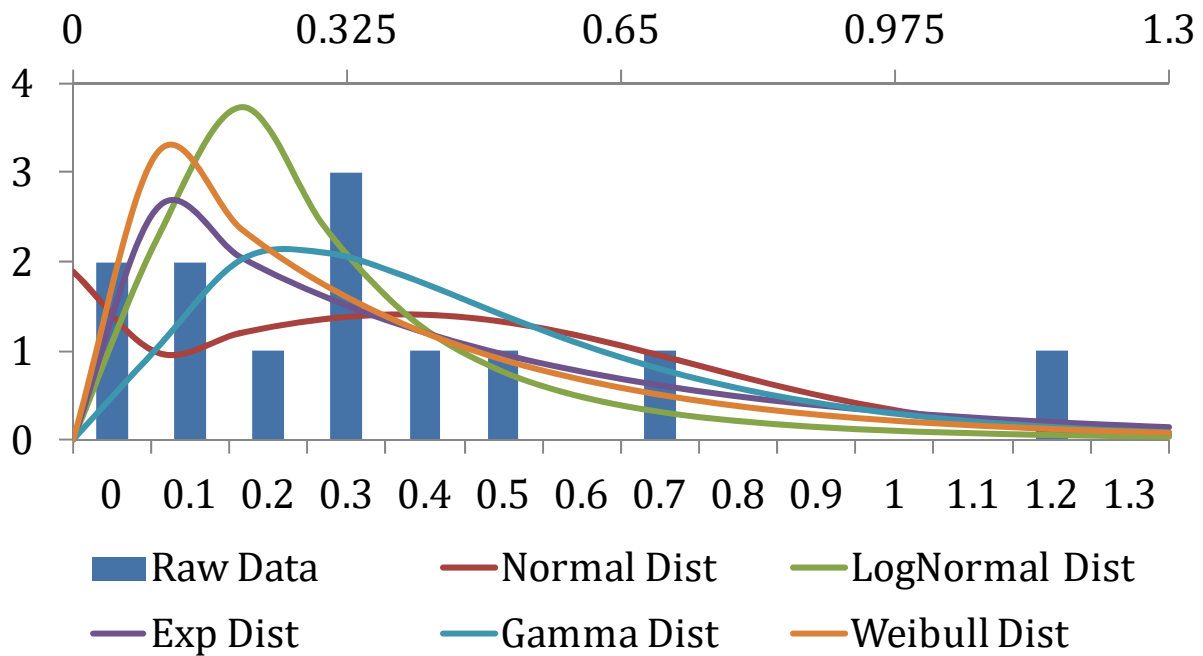


Figure 48: Histogram, NO2, Multivariate/Ovens

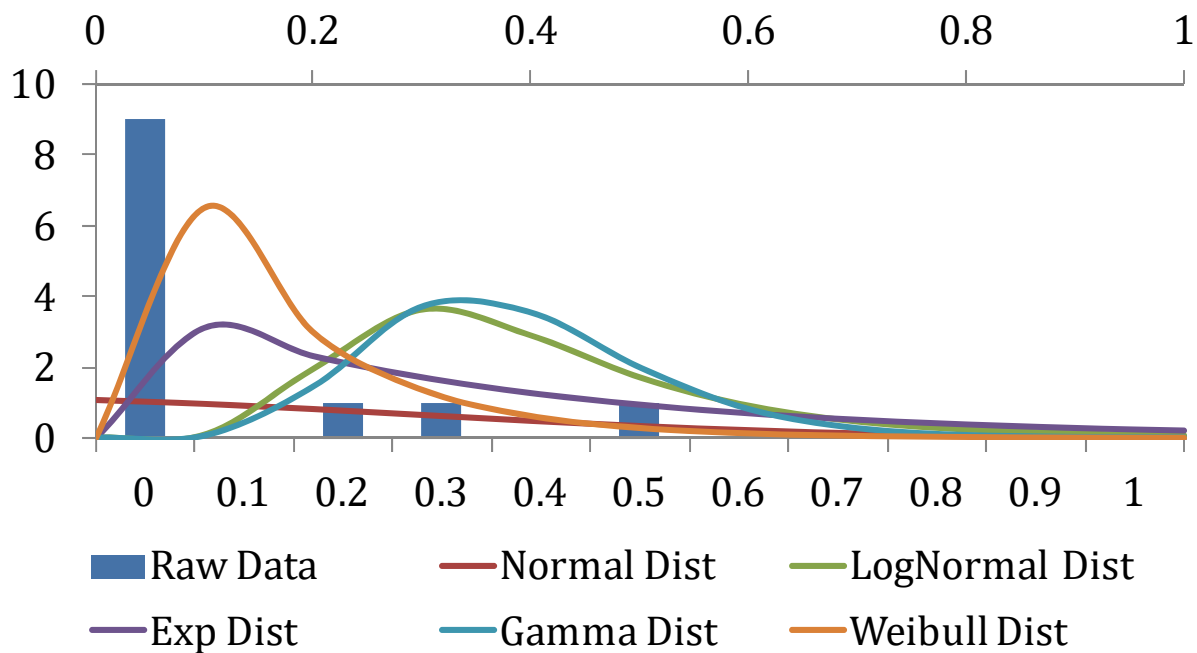


Figure 49: Histogram, NOx, Multivariate/Ovens

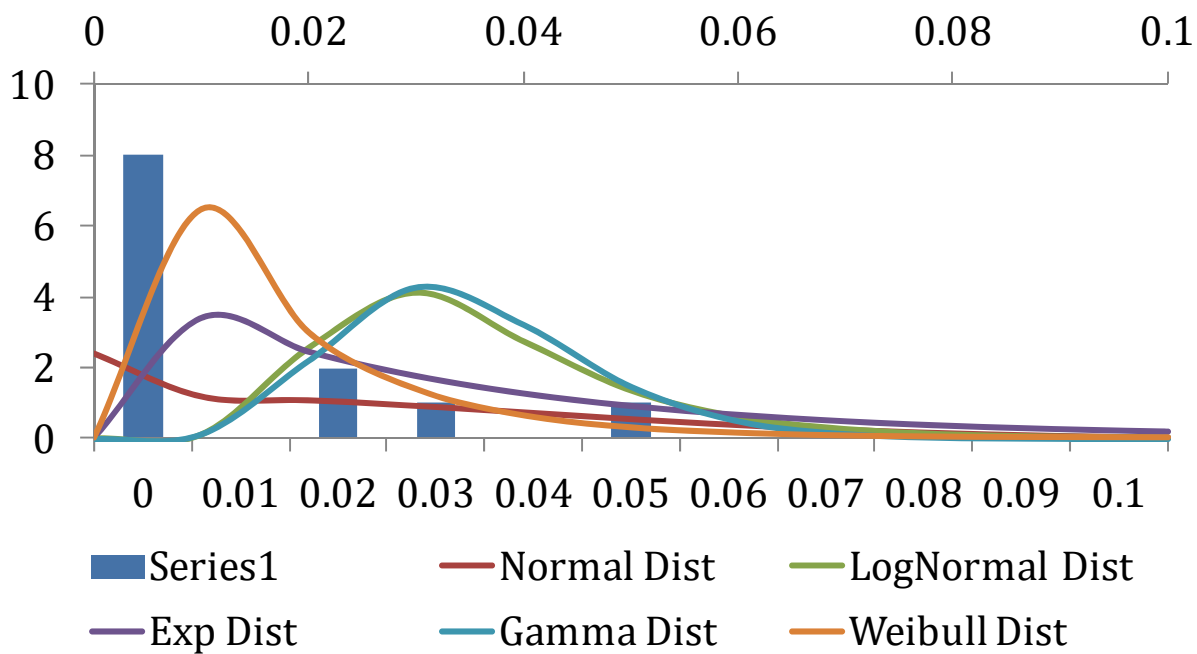


Figure 50: Histogram, HCHO, Bivariate/Ovens

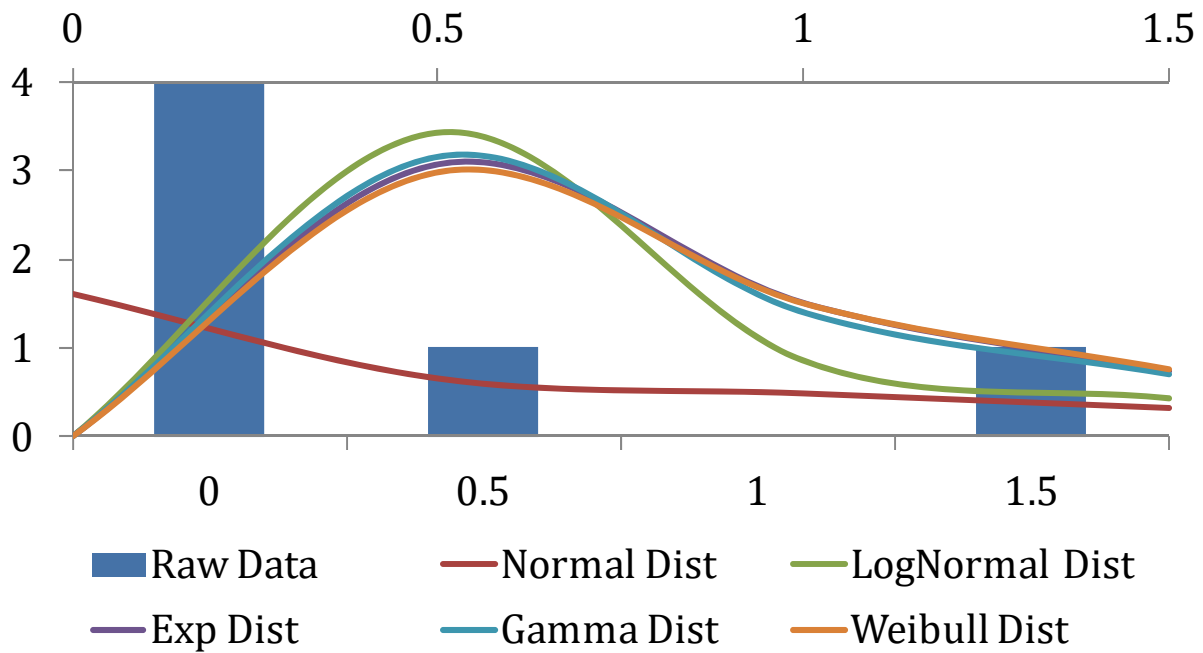


Figure 51: Histogram, CO, Full/Furnaces

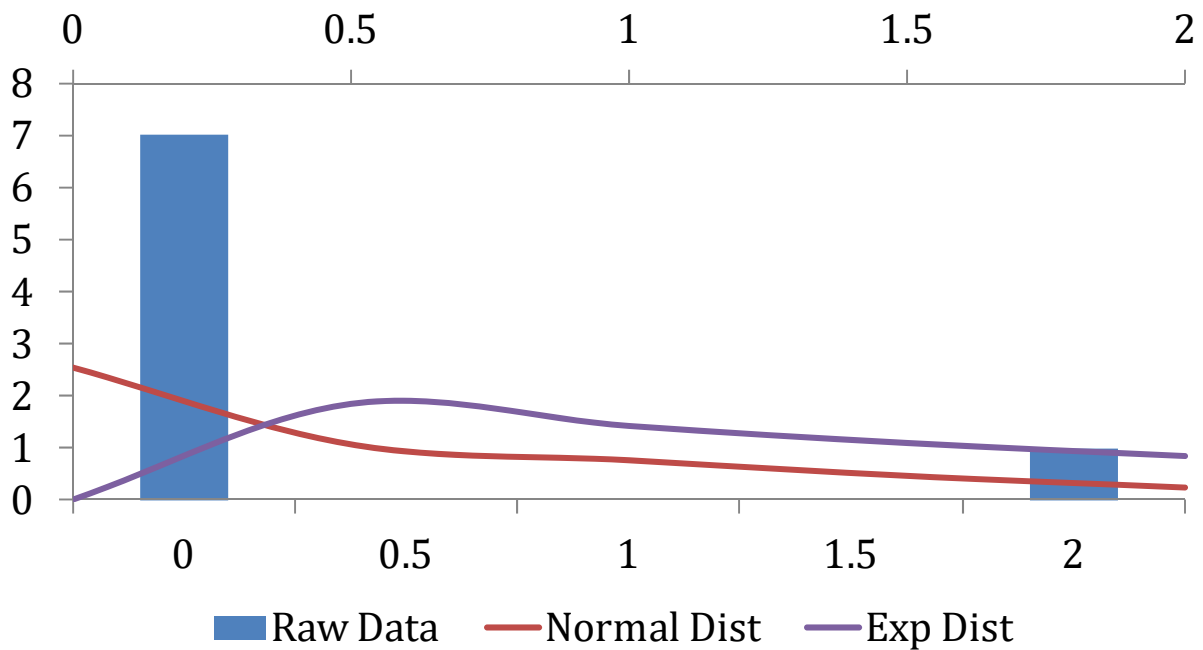


Figure 52: Histogram, CO, End/Furnaces

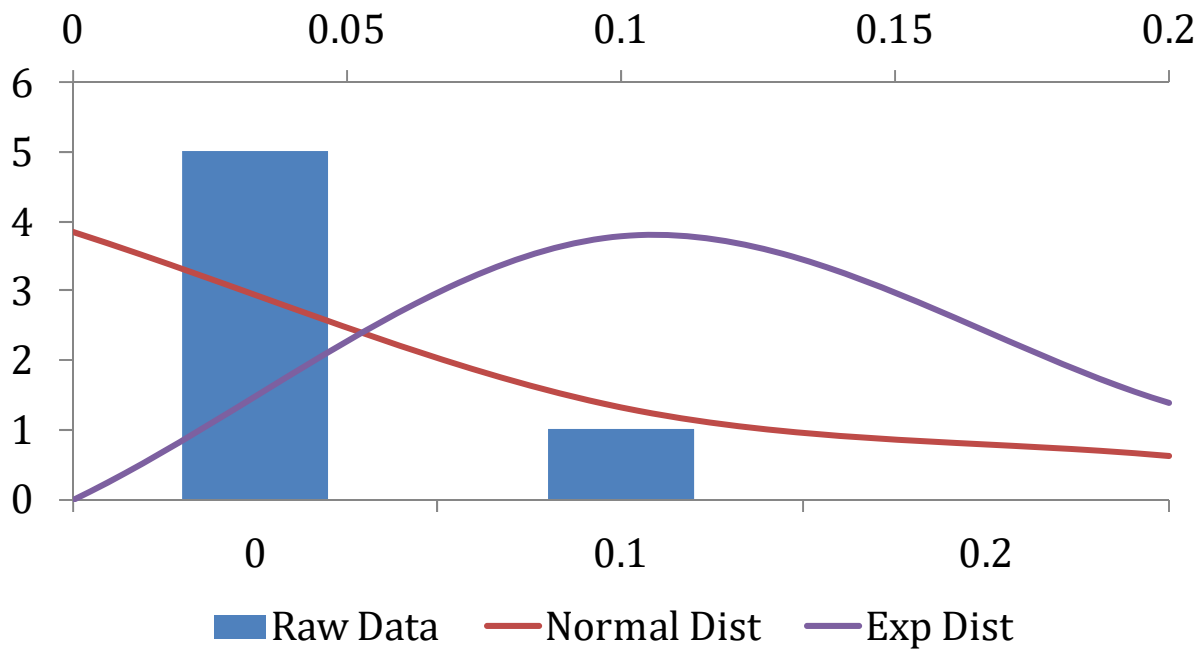


Figure 53: Histogram, NO2/Furnaces

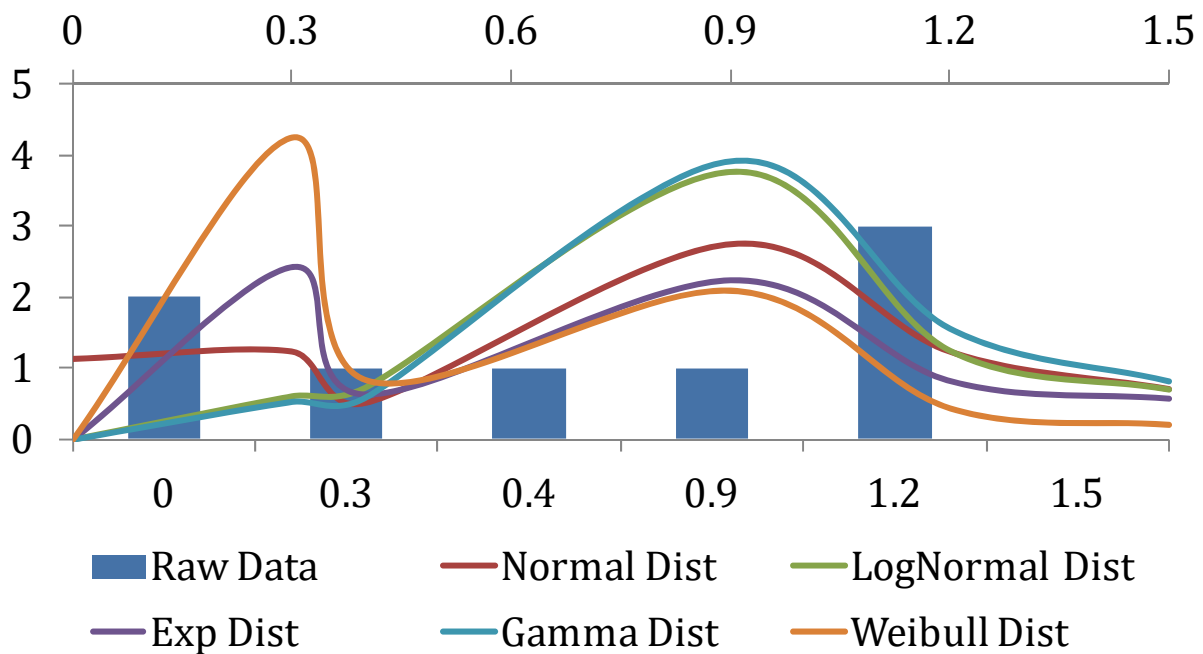


Figure 54: Histogram, NOx/Furnaces

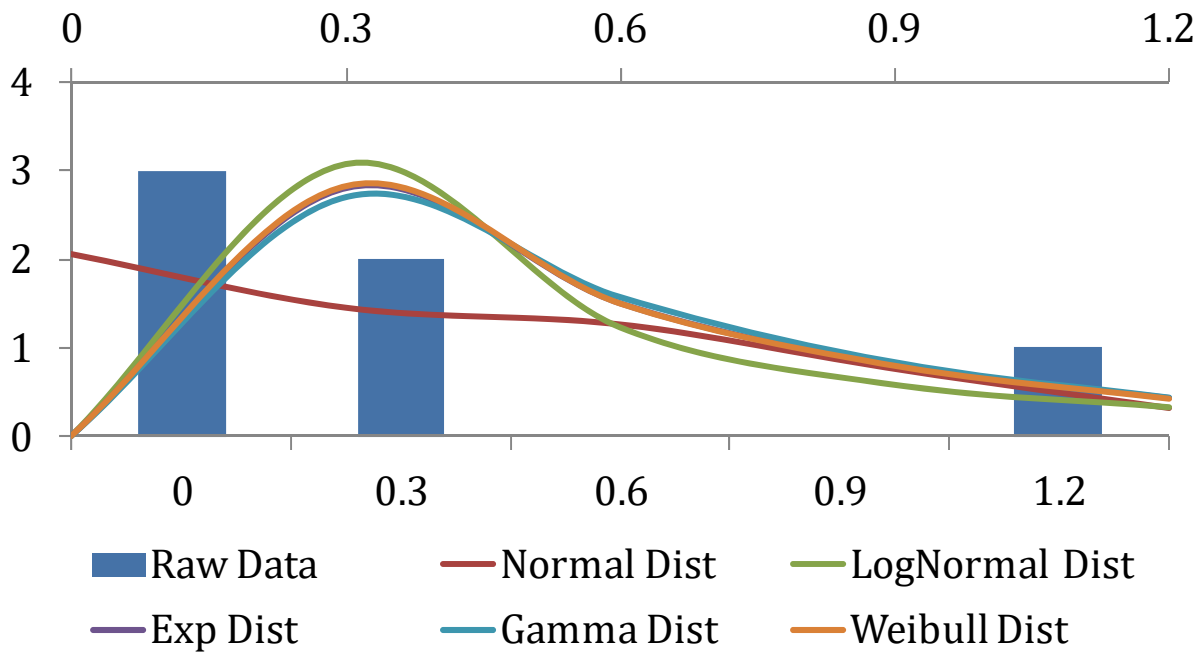


Figure 55: Histogram, CO/Storage Water Heaters

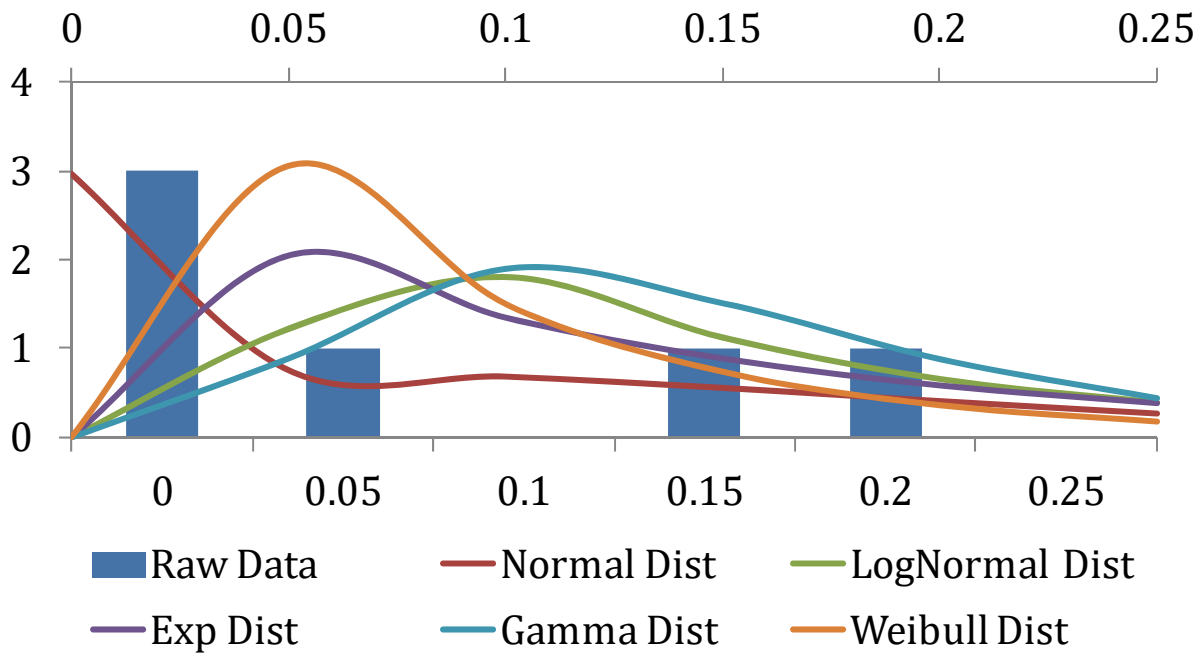


Figure 56: Histogram, NO2/Storage Water Heaters

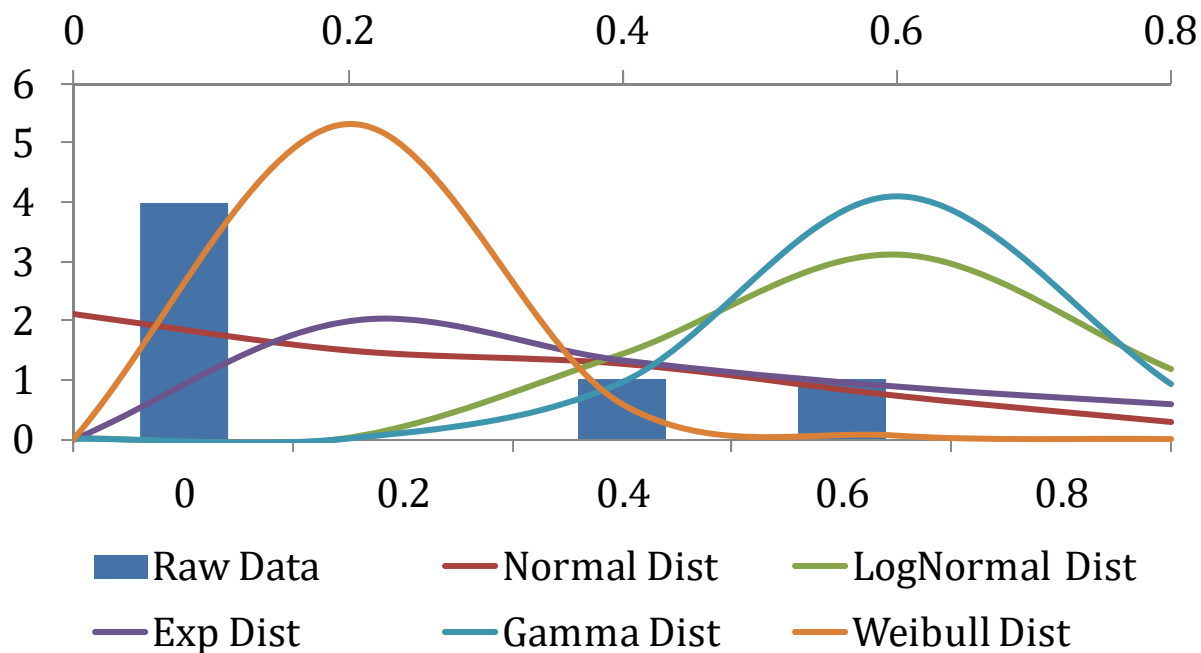


Figure 57: Histogram, NOx/Storage Water Heaters

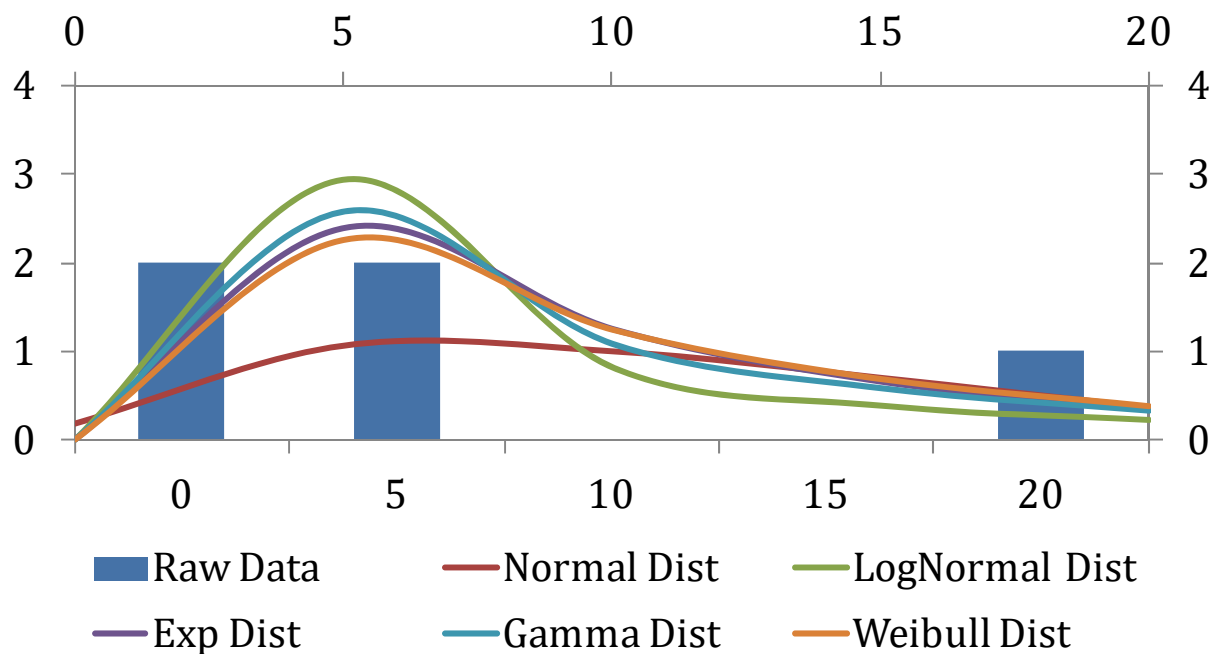


Figure 58: Histogram, CO Full, Multivariate/Tankless Water Heaters

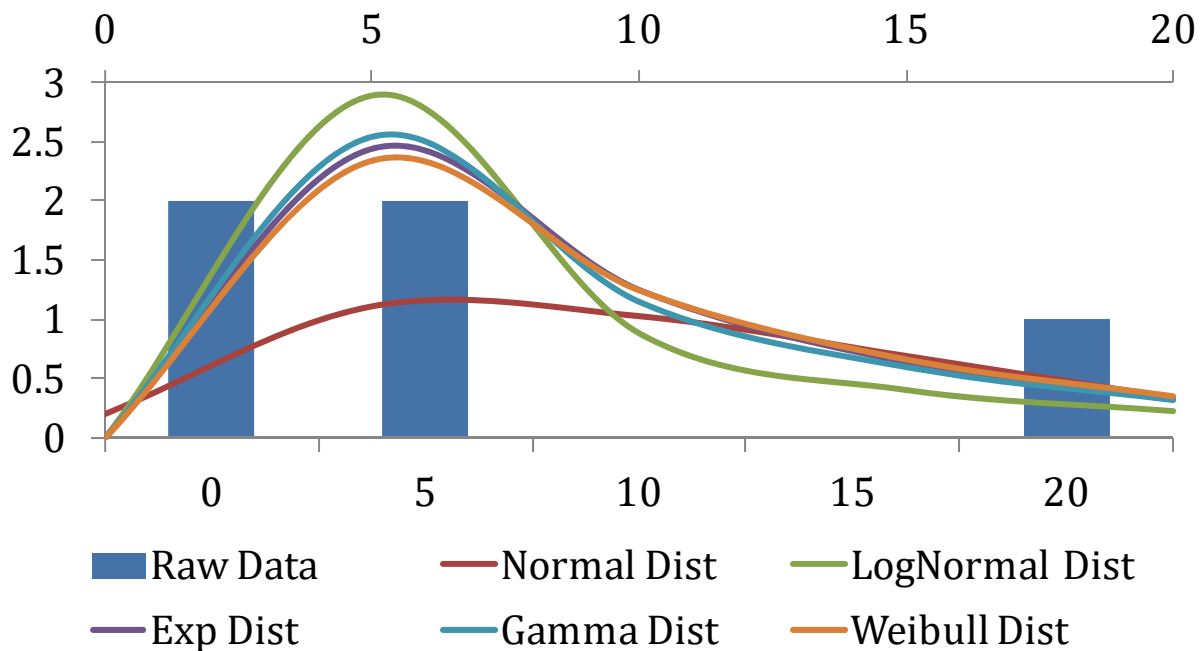


Figure 59: Histogram, CO End, Multivariate/Tankless Water Heaters

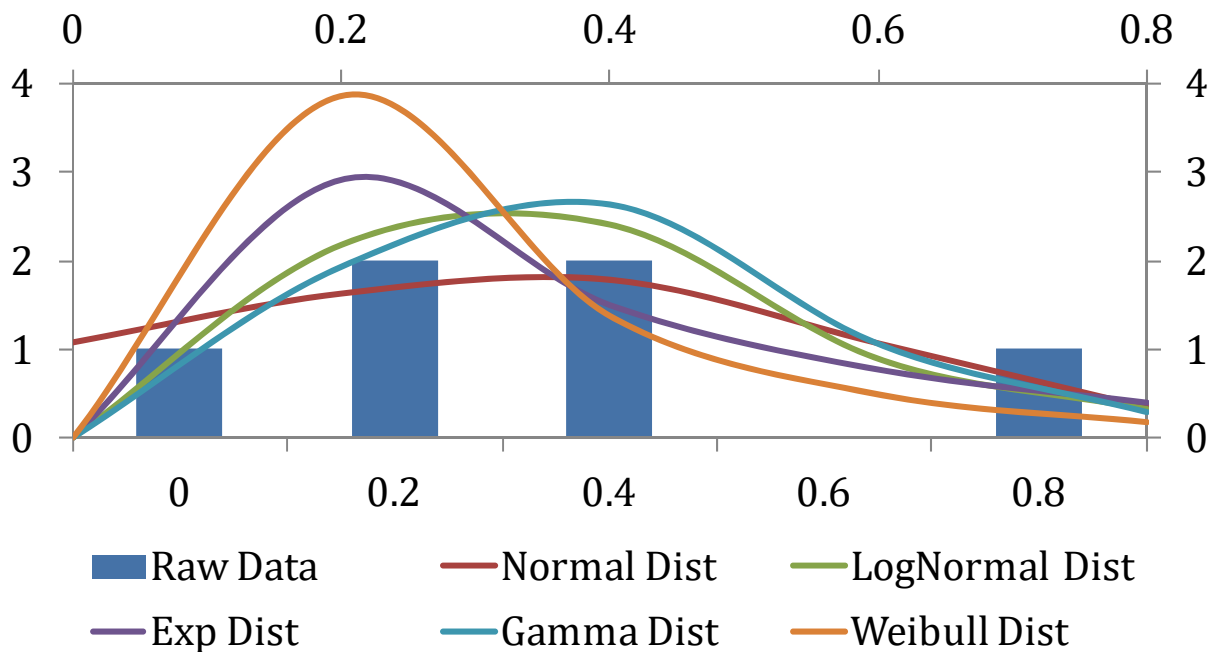


Figure 60: Histogram, NO2, Multivariate/Tankless Water Heaters

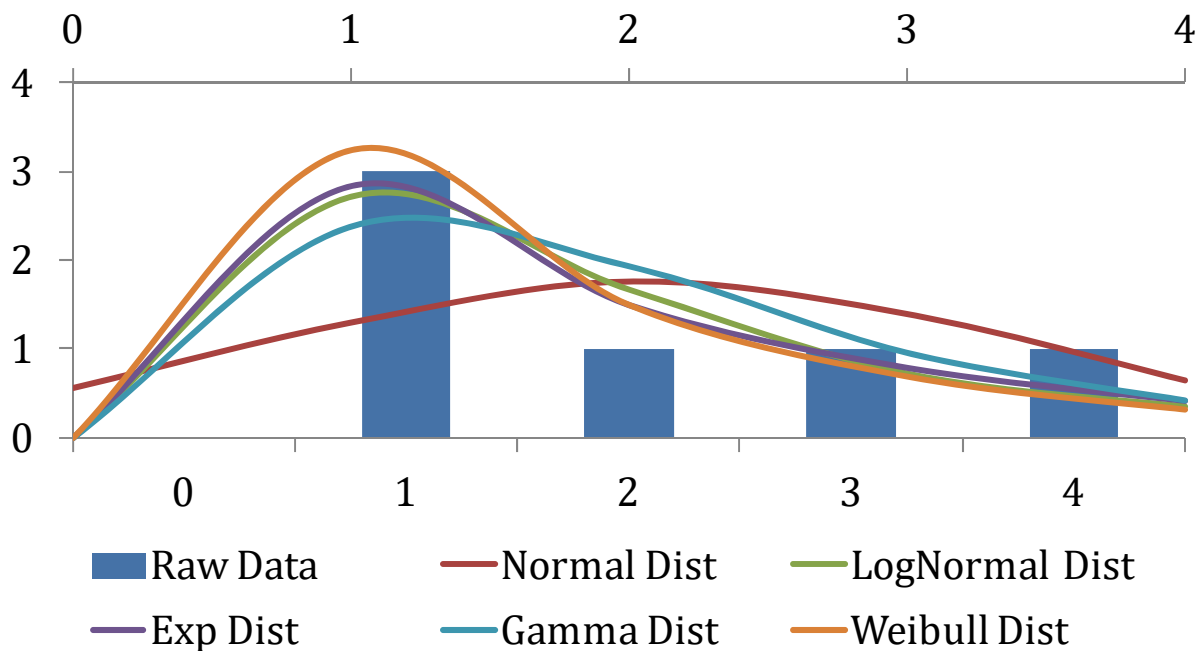


Figure 61: Histogram NOx, Multivariate/Tankless Water Heaters

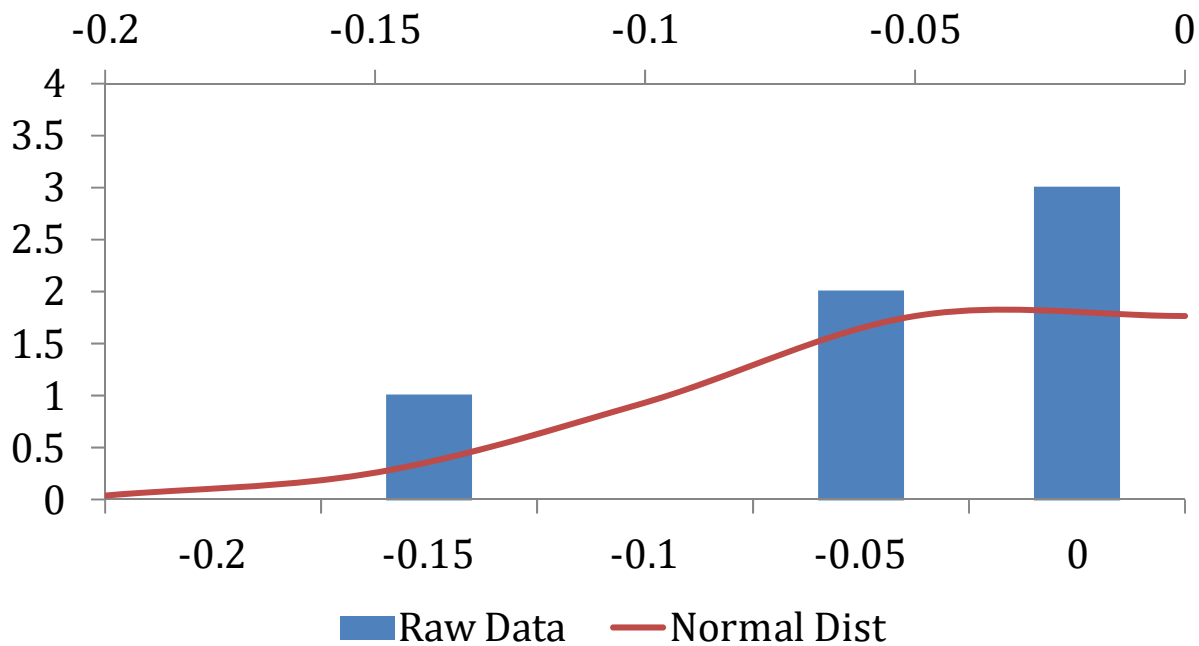


Figure 62: Histogram, HCHO, Bivariate/Tankless Water Heaters

XXII.D Distribution Cumulative Probability Plots

Horizontal axes in the following figures are all changes in emission rates (ng/J) per change of 25 in WN. Vertical axes are cumulative probabilities, with the maximum at unity equivalent to 100% probability.

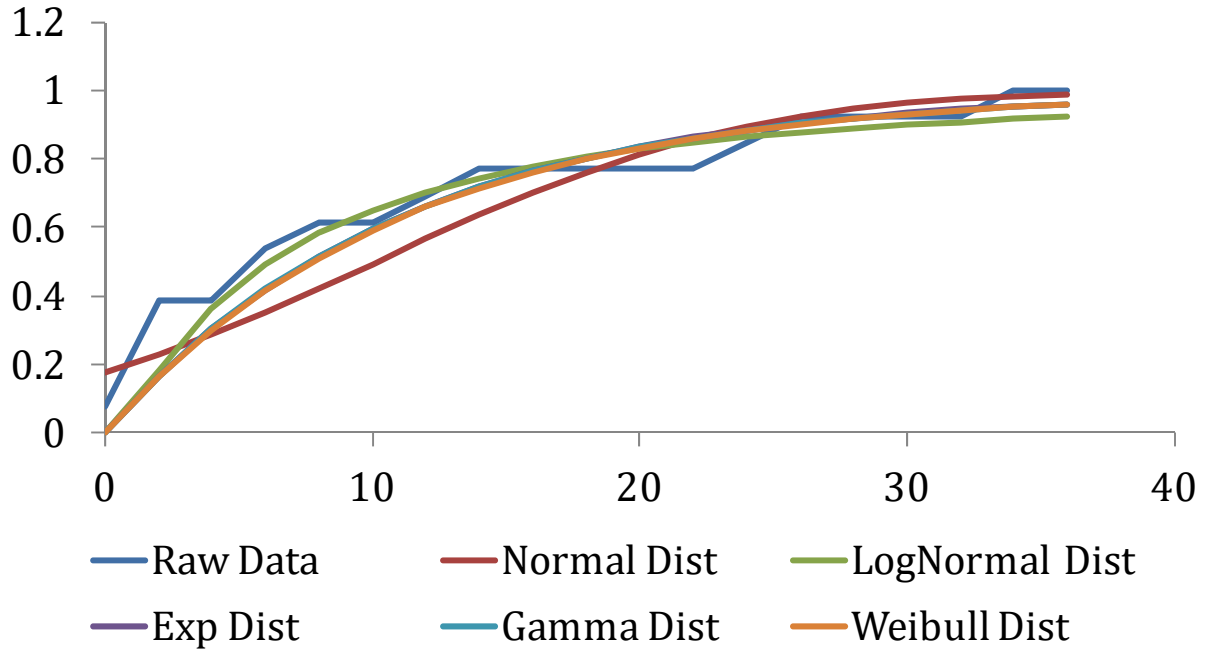


Figure 63: Cumulative Probability Functions, CO, Full/Cooktops

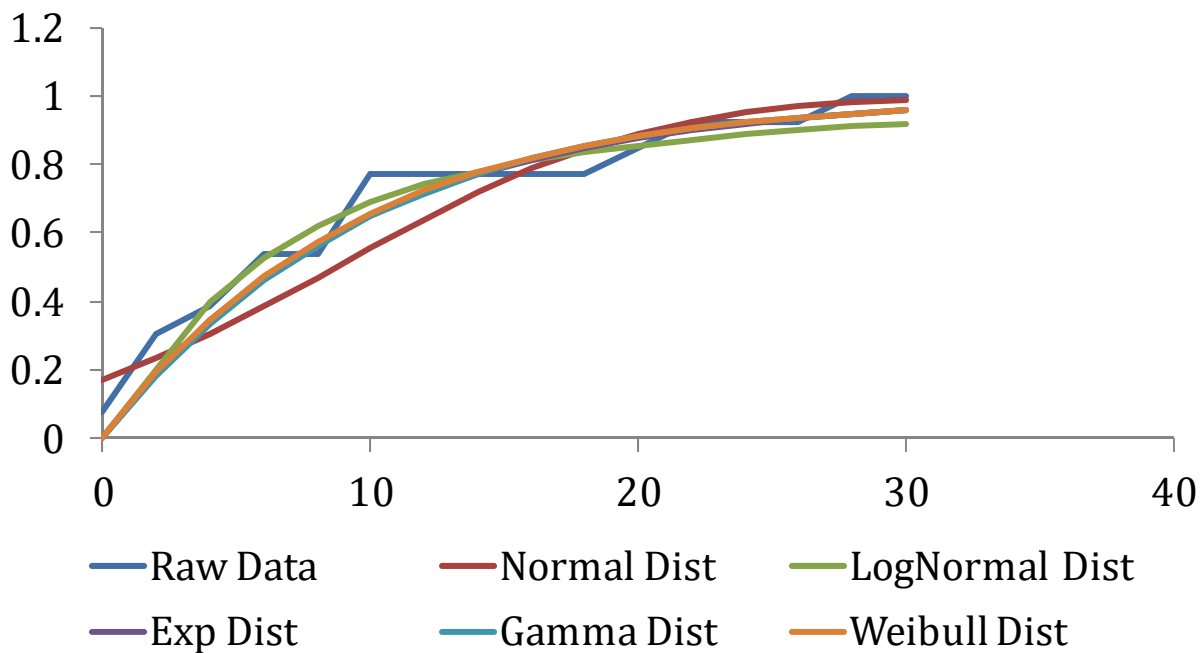


Figure 64: Cumulative Probability Functions, CO, End/Cooktops

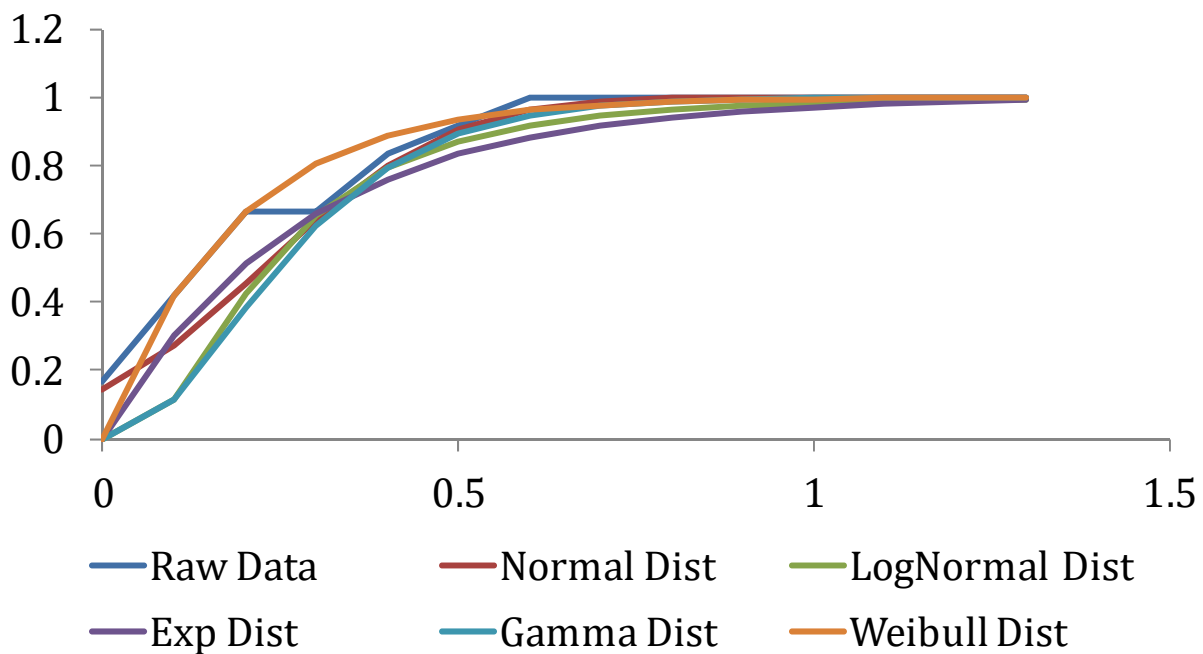


Figure 65: Cumulative Probability Functions, NO2, Full/Cooktops

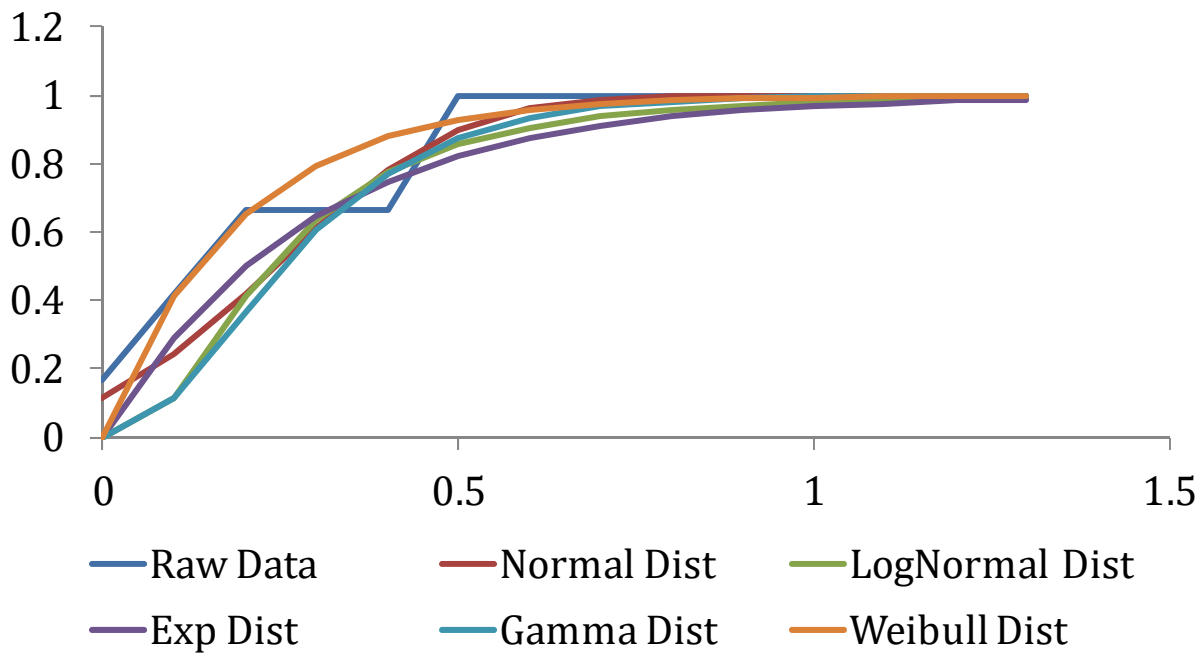


Figure 66: Cumulative Probability Functions, NO₂, End/Cooktops

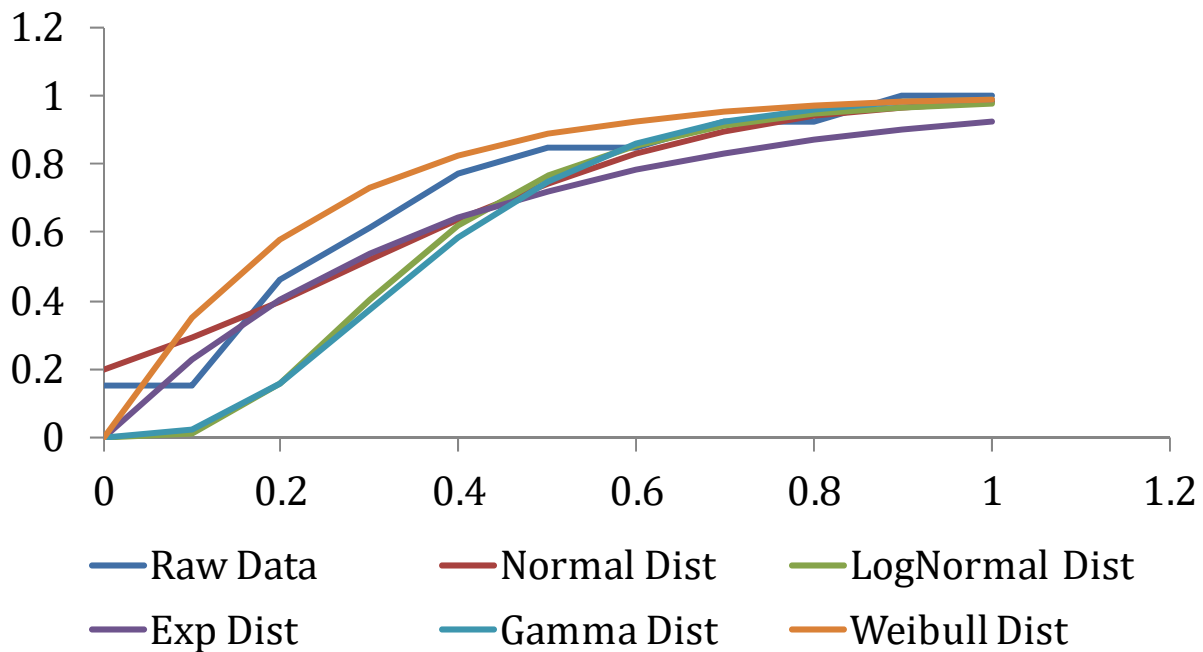


Figure 67: Cumulative Probability Functions, NO_x, Full/Cooktops

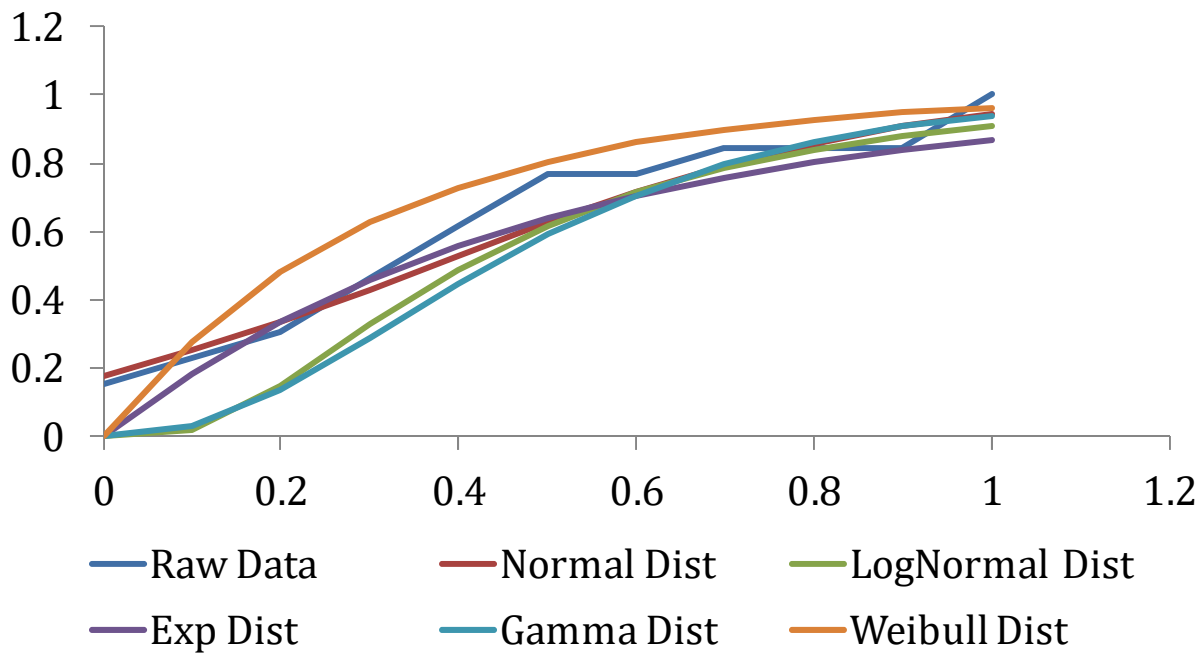


Figure 68: Cumulative Probability Functions, NOx, End/Cooktops

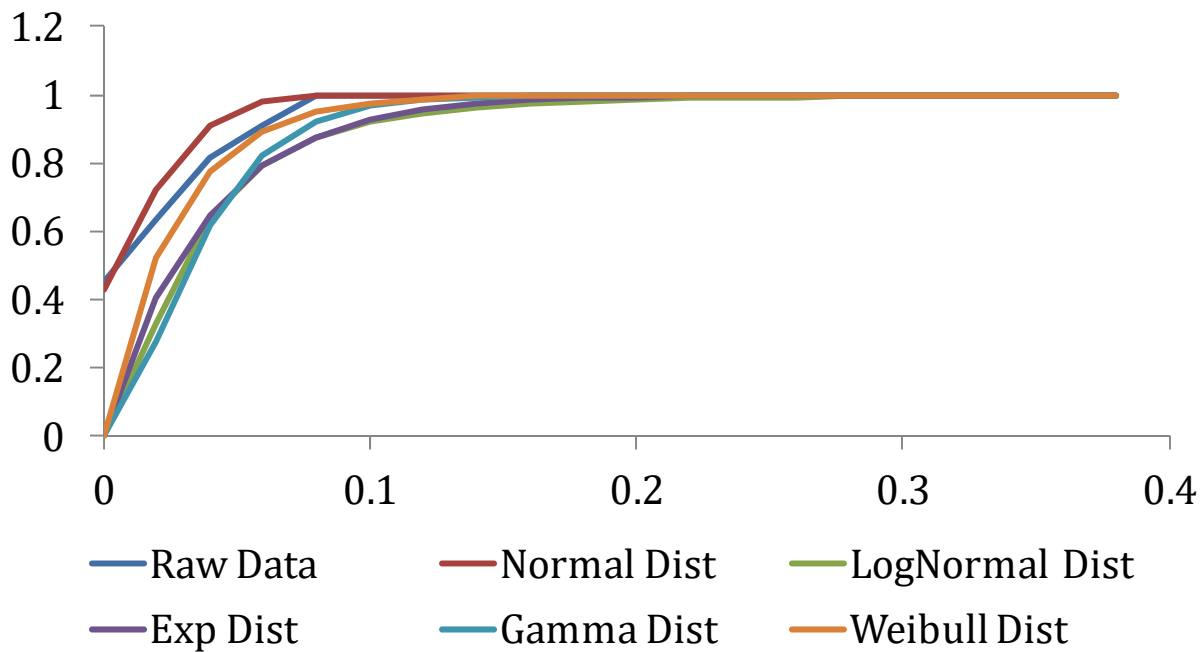


Figure 69: Cumulative Probability Functions, HCHO/Cooktops

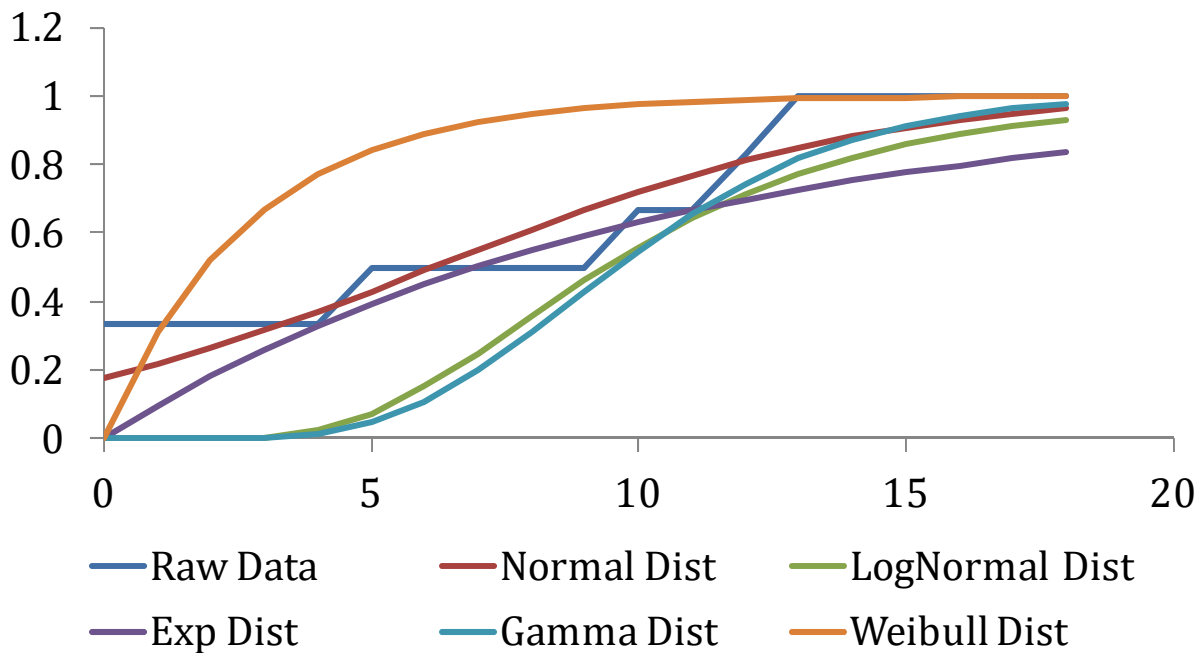


Figure 70: Cumulative Probability Functions, CO, Full/Broilers

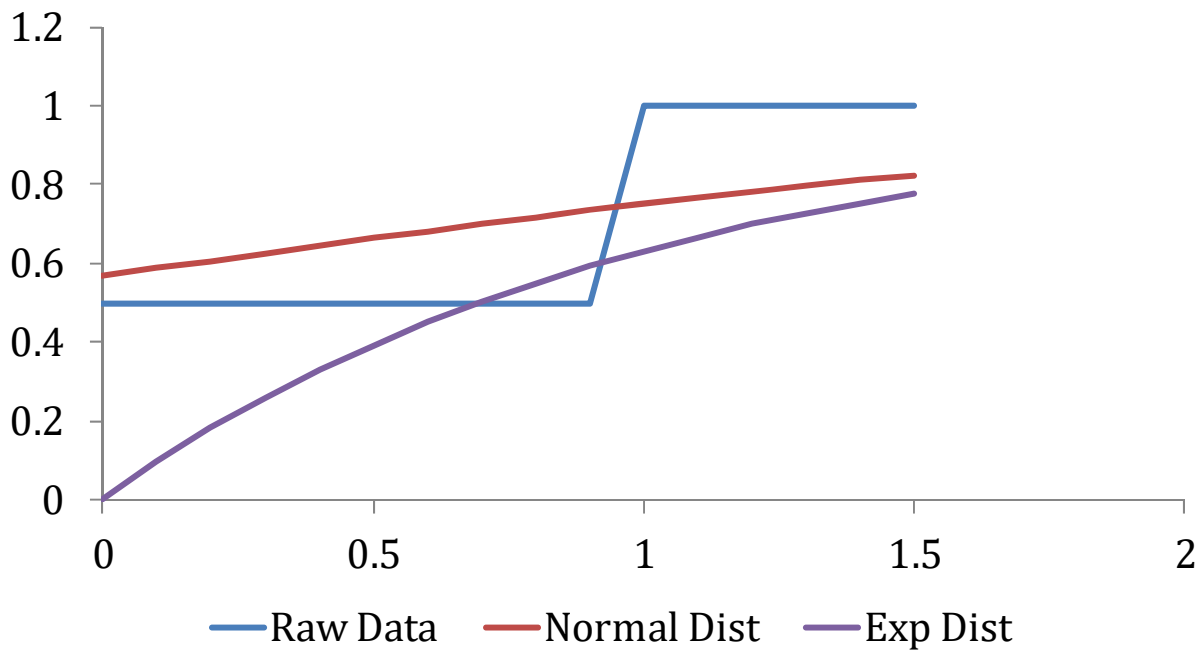


Figure 71: Cumulative Probability Functions, CO, End/Broilers

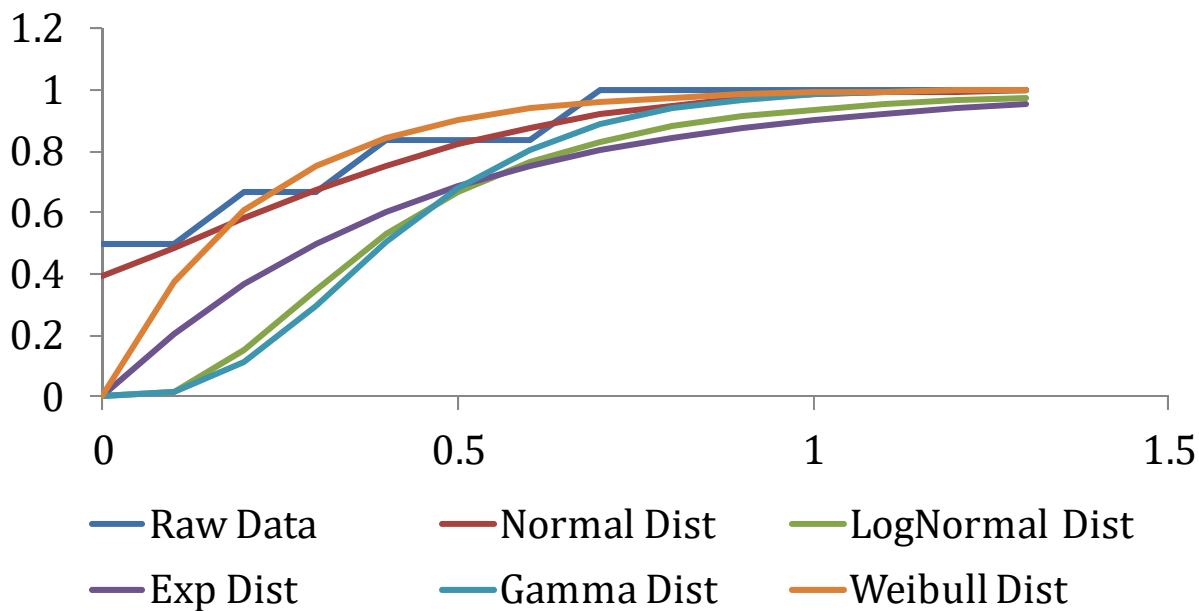


Figure 72: Cumulative Probability Functions, NO2/Broilers

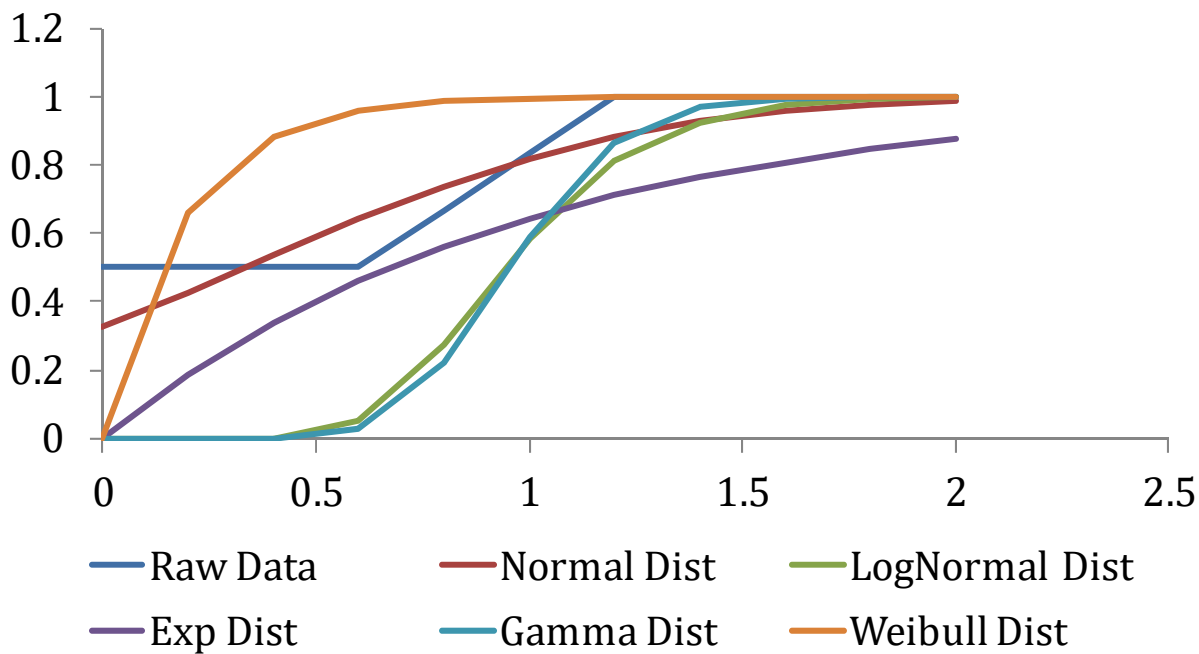


Figure 73: Cumulative Probability Functions, NOx/Broilers

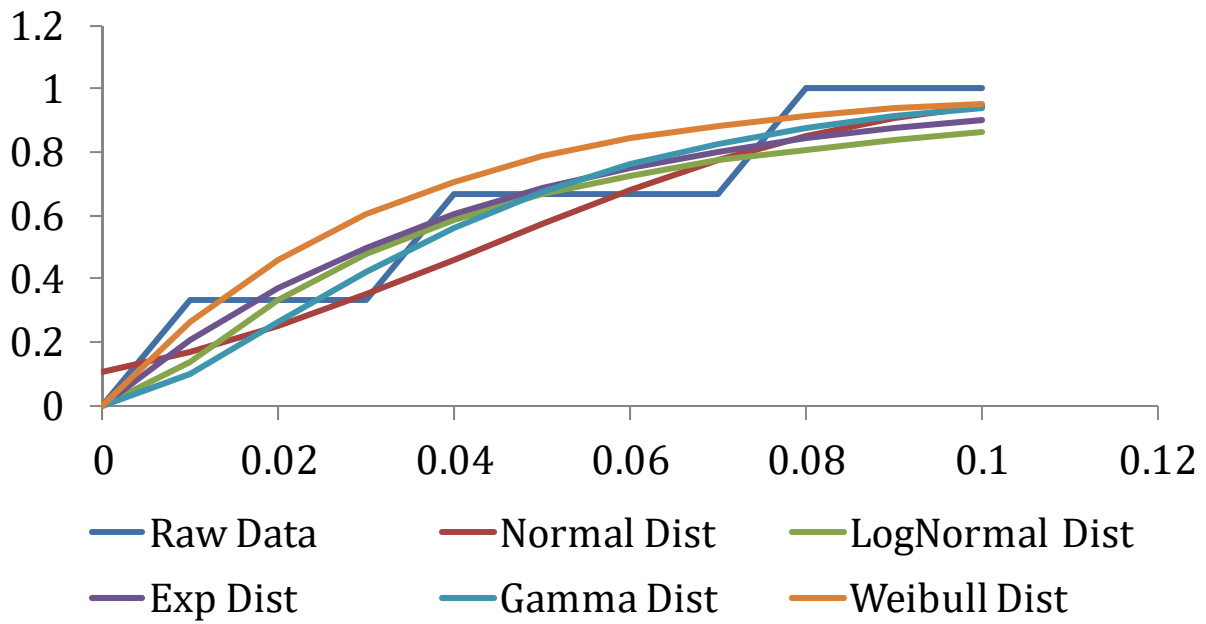


Figure 74: Cumulative Probability Functions, HCHO/Broilers

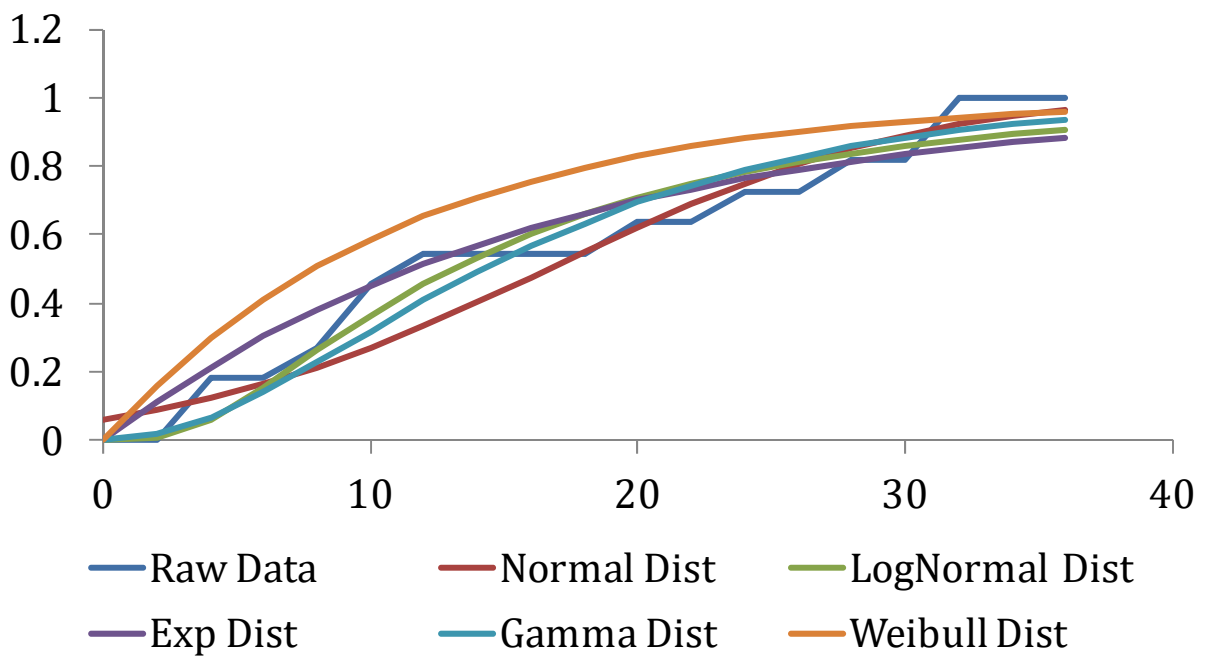


Figure 75: Cumulative Probability Functions, CO, Bivariate/Ovens

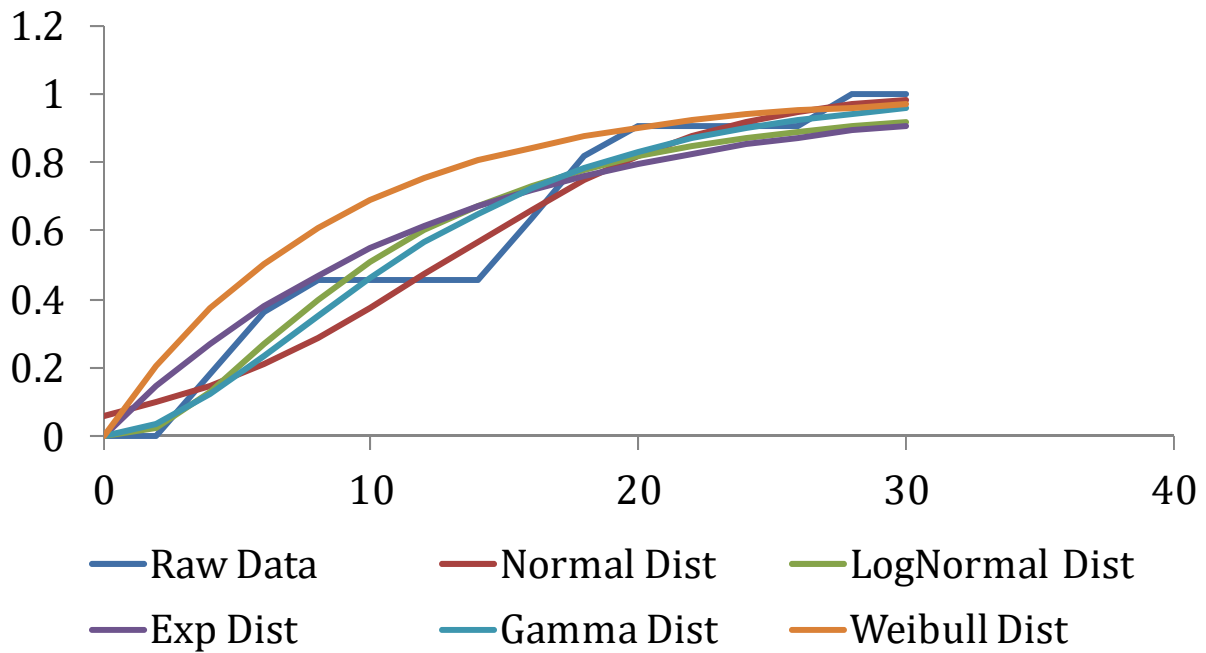


Figure 76: Cumulative Probability Functions, CO, Multivariate/Ovens

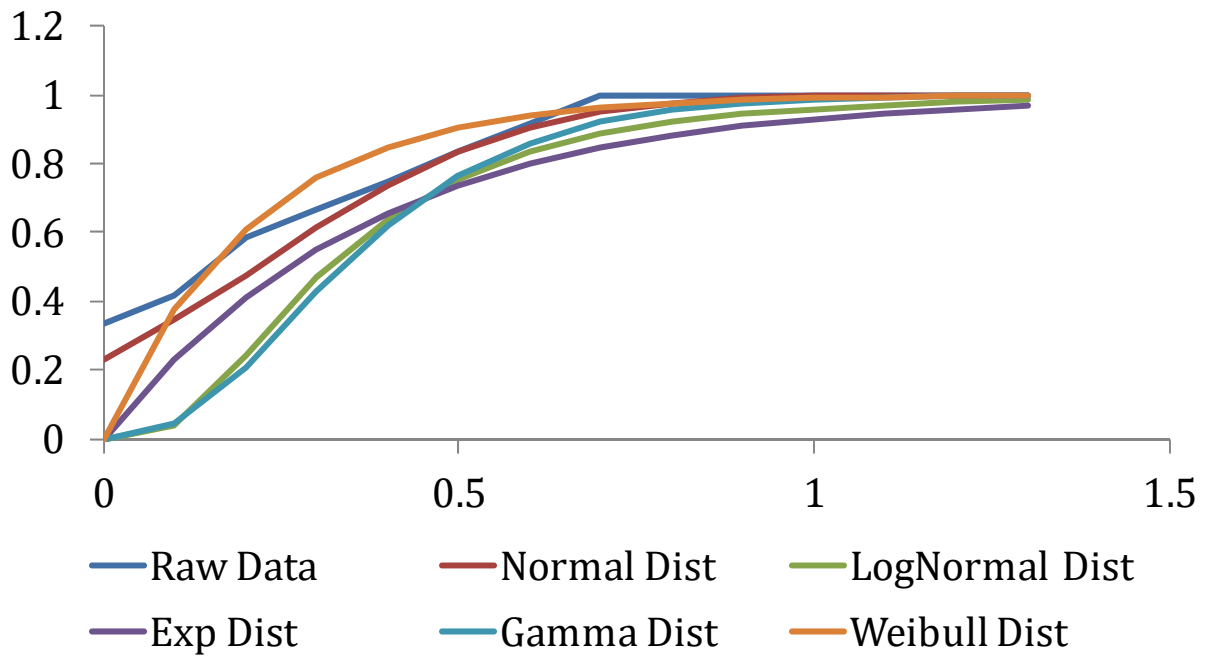


Figure 77: Cumulative Probability Functions, NO2, Bivariate/Ovens

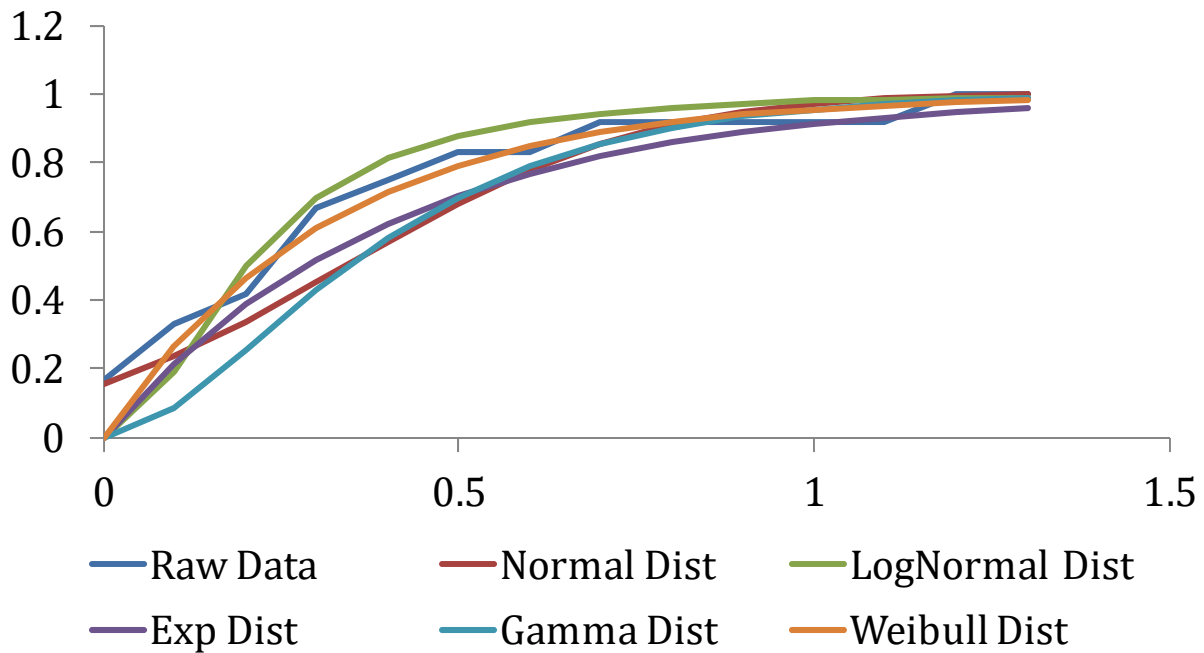


Figure 78: Cumulative Probability Functions, NO2, Multivariate/Ovens

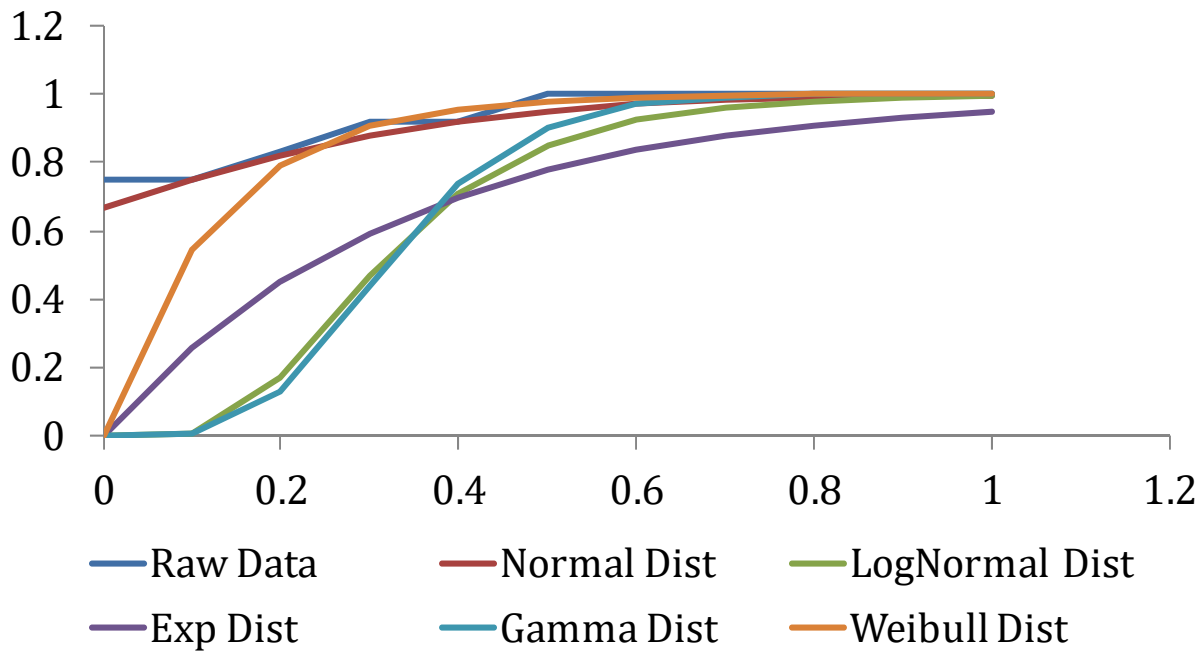


Figure 79: Cumulative Probability Distributions, NOx, Multivariate/Ovens

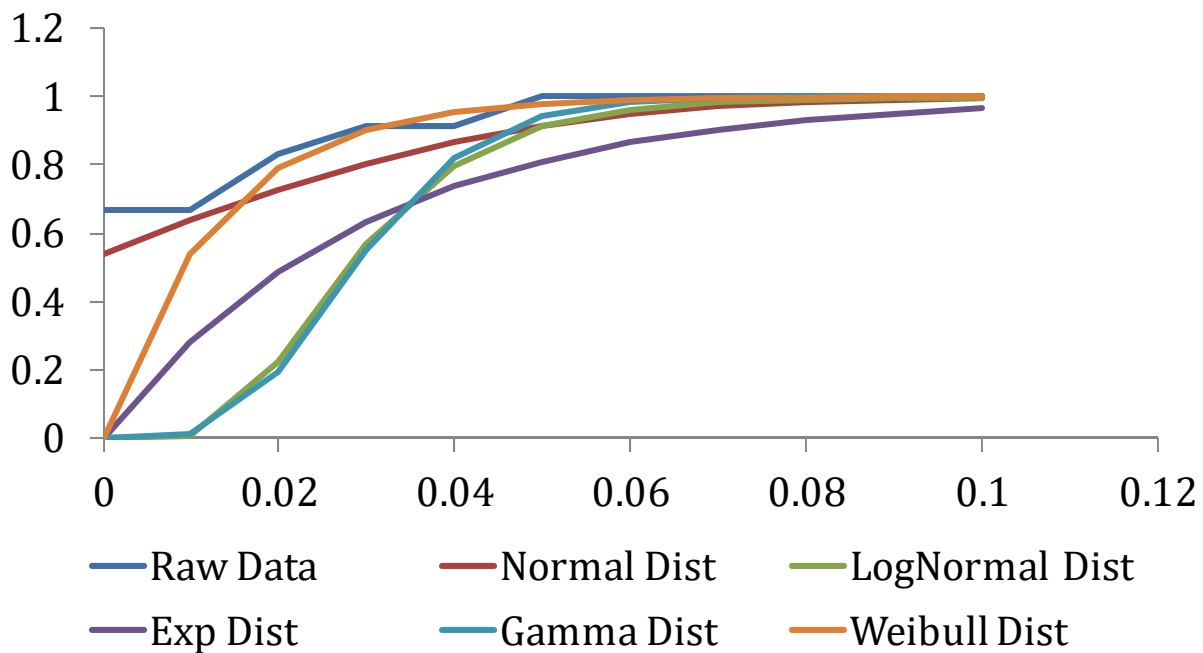


Figure 80: Cumulative Probability Distributions, HCHO, Bivariate/Ovens

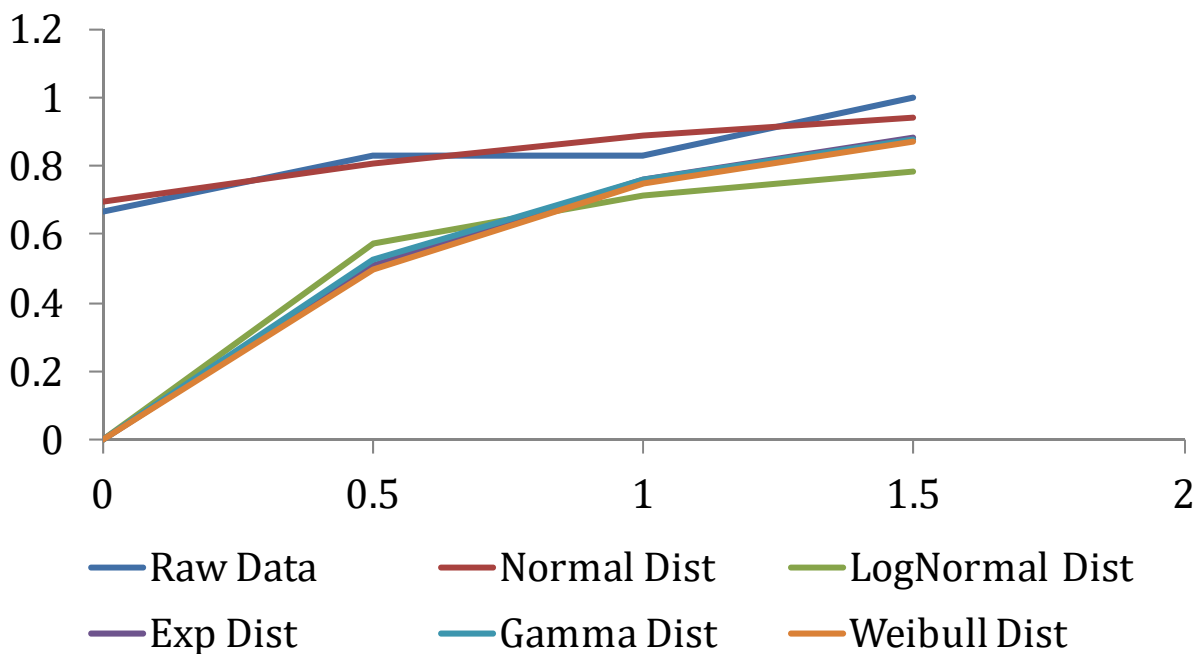


Figure 81: Cumulative Probability Functions, CO, Full/Furnaces

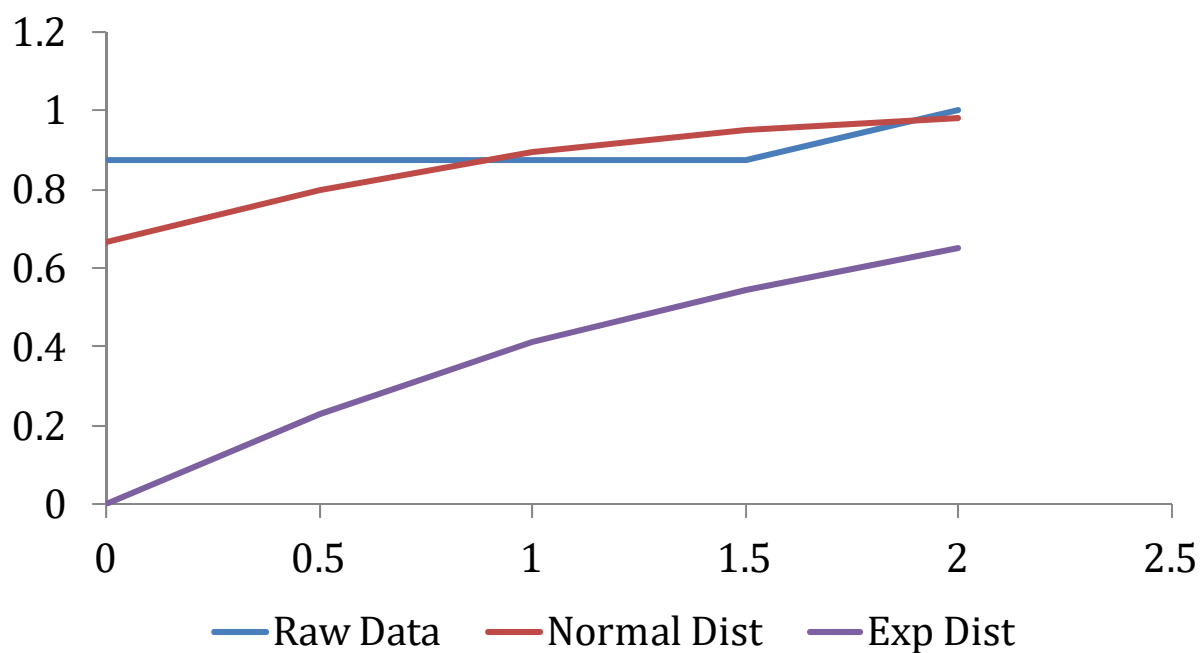


Figure 82: Cumulative Probability Functions, CO, End/Furnaces

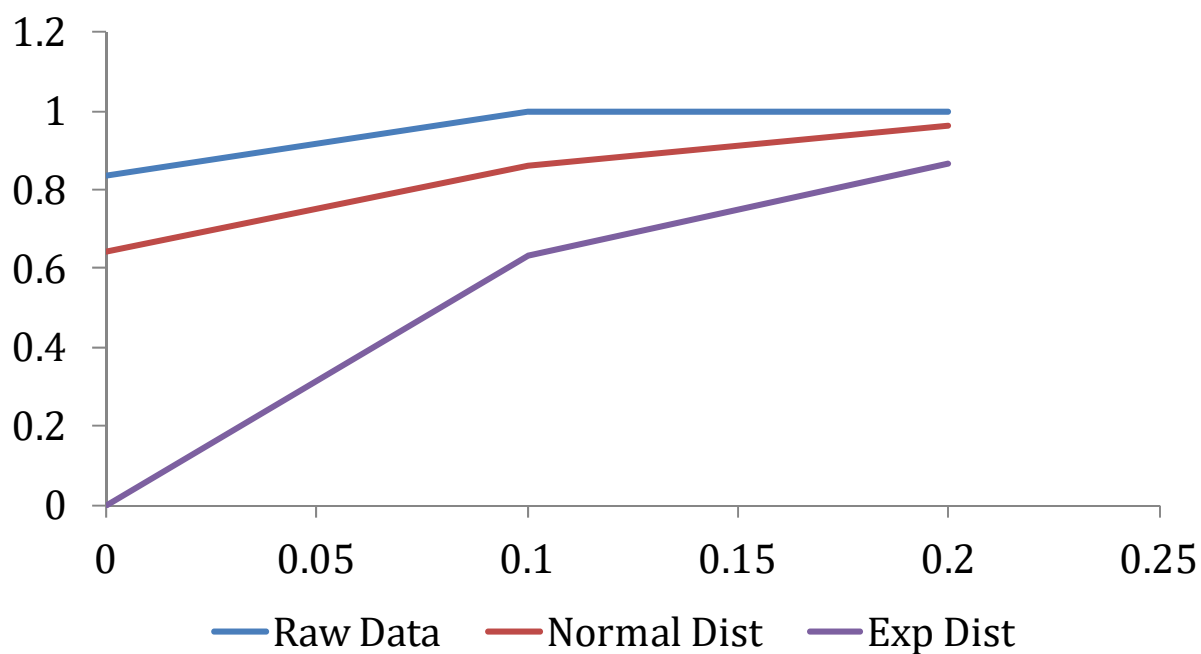


Figure 83: Cumulative Probability Functions, NO2/Furnaces

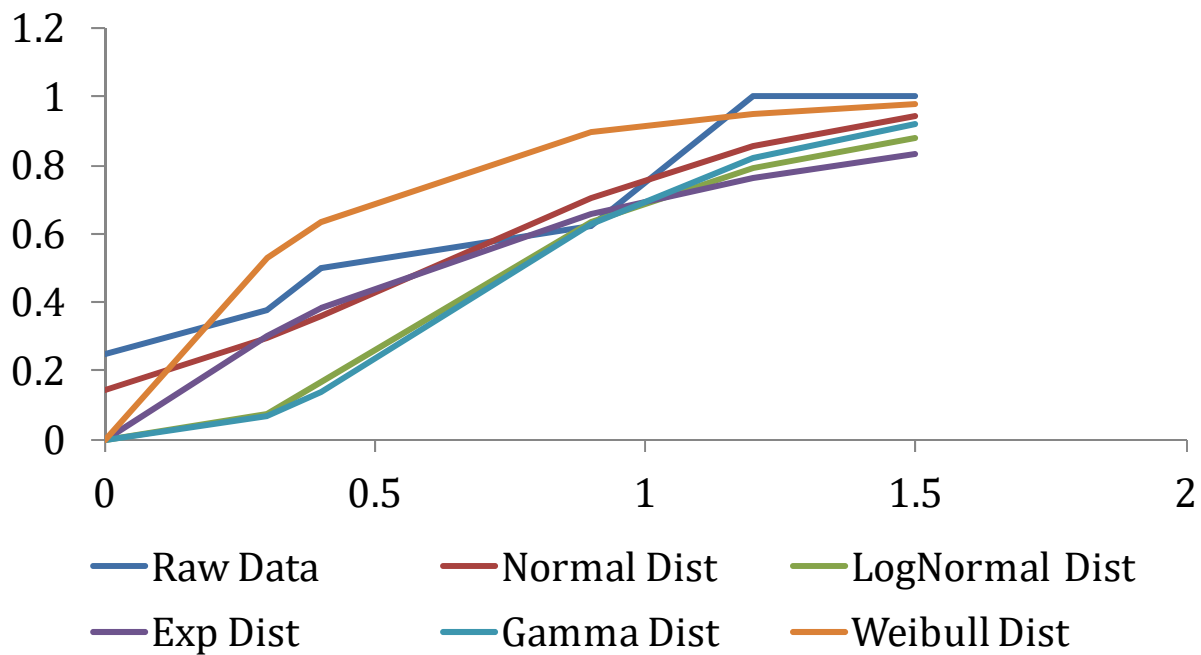


Figure 84: Cumulative Probability Functions, NOx/Furnaces

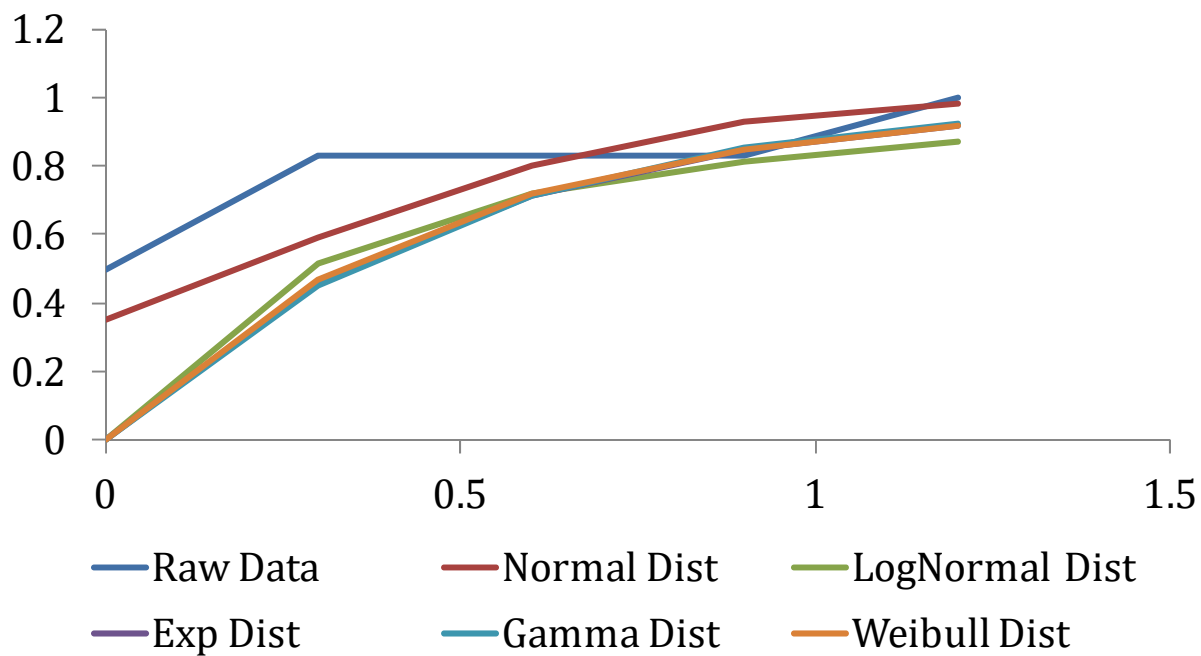


Figure 85: Cumulative Probability Functions, CO/Storage Water Heaters

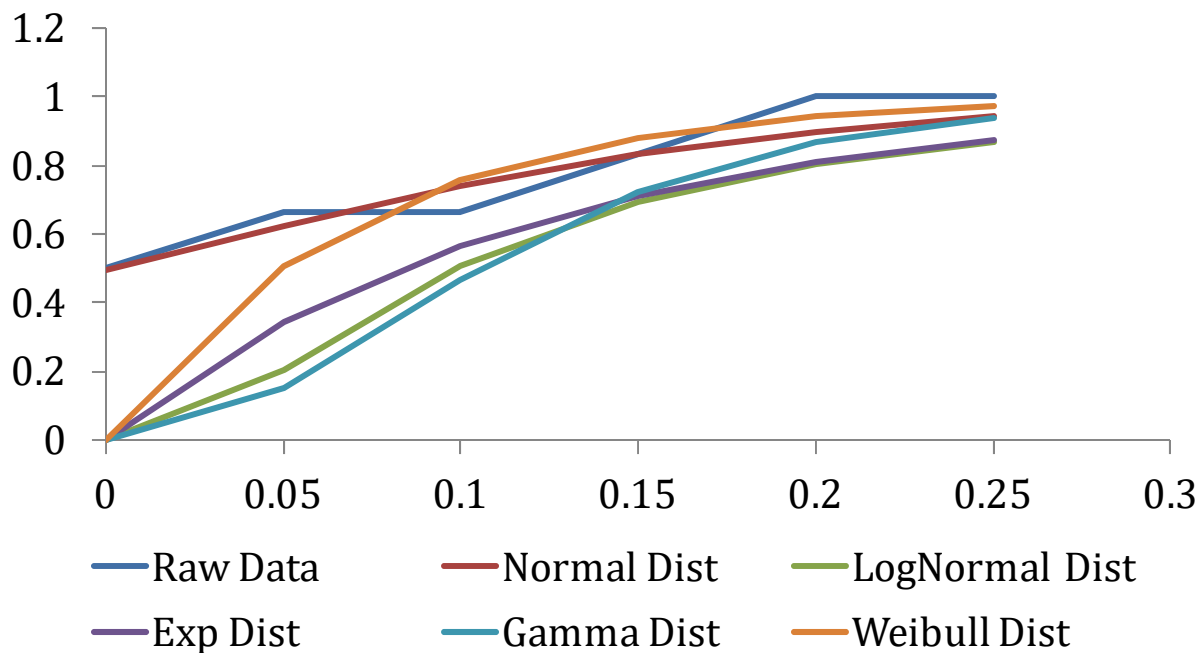


Figure 86: Cumulative Probability Functions, NO2/Storage Water Heaters

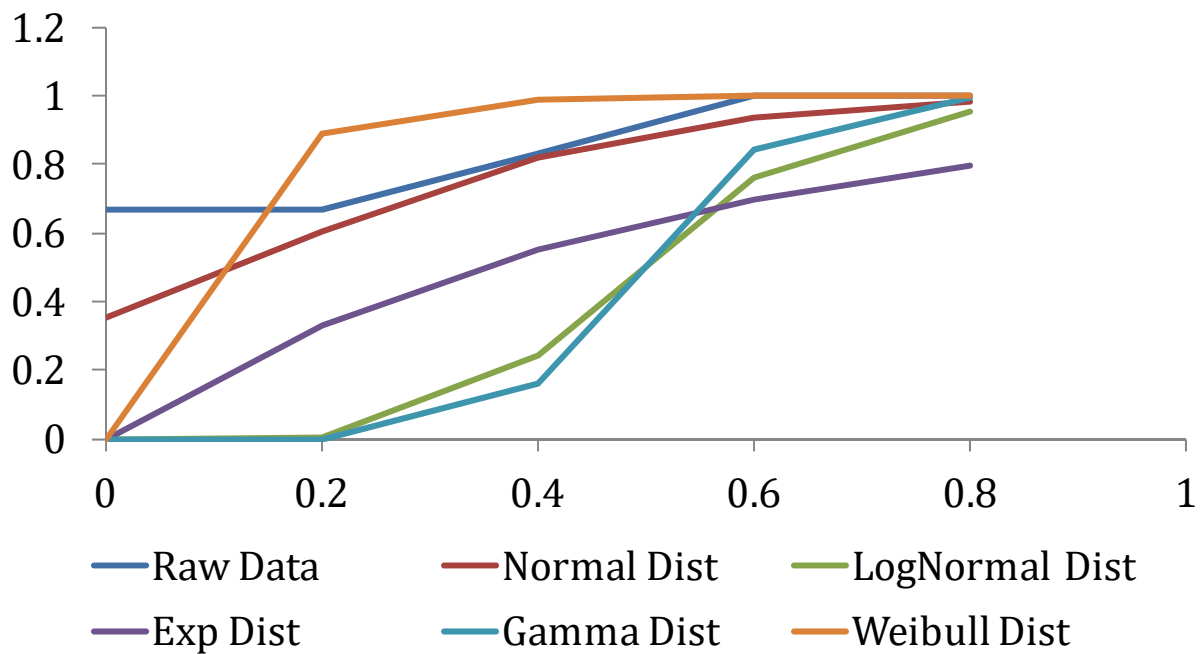


Figure 87: Cumulative Probability Functions, NOx/Storage Water Heaters

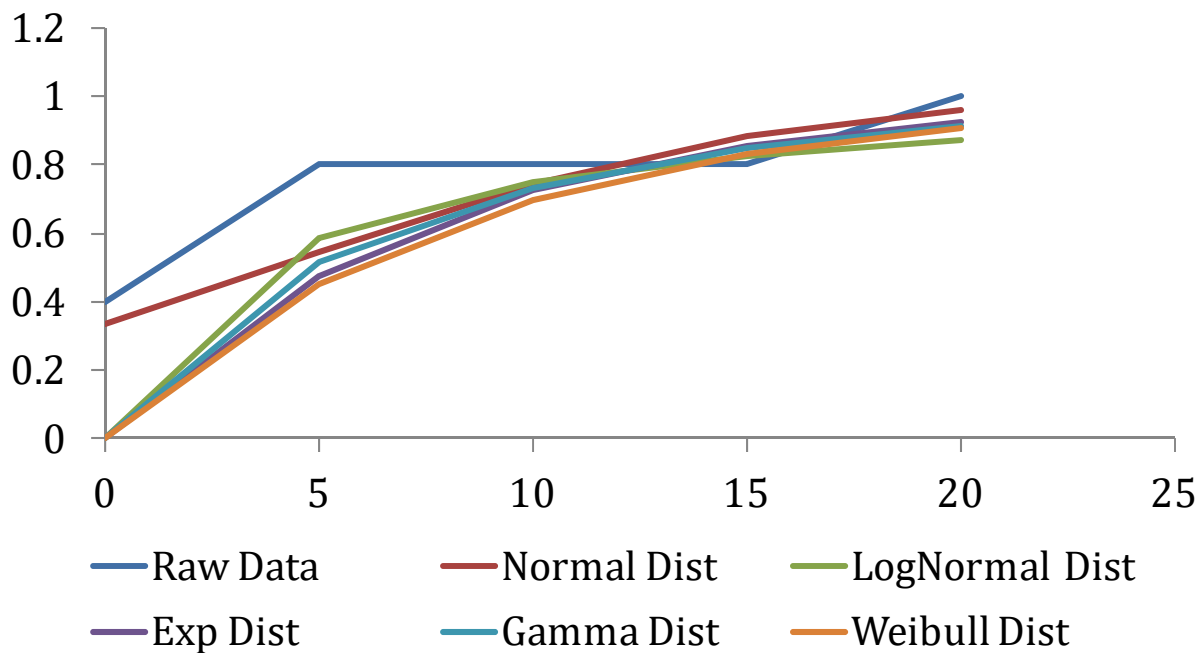


Figure 88: Cumulative Probability Functions, CO Full, Multivariate/Tankless Water Heaters

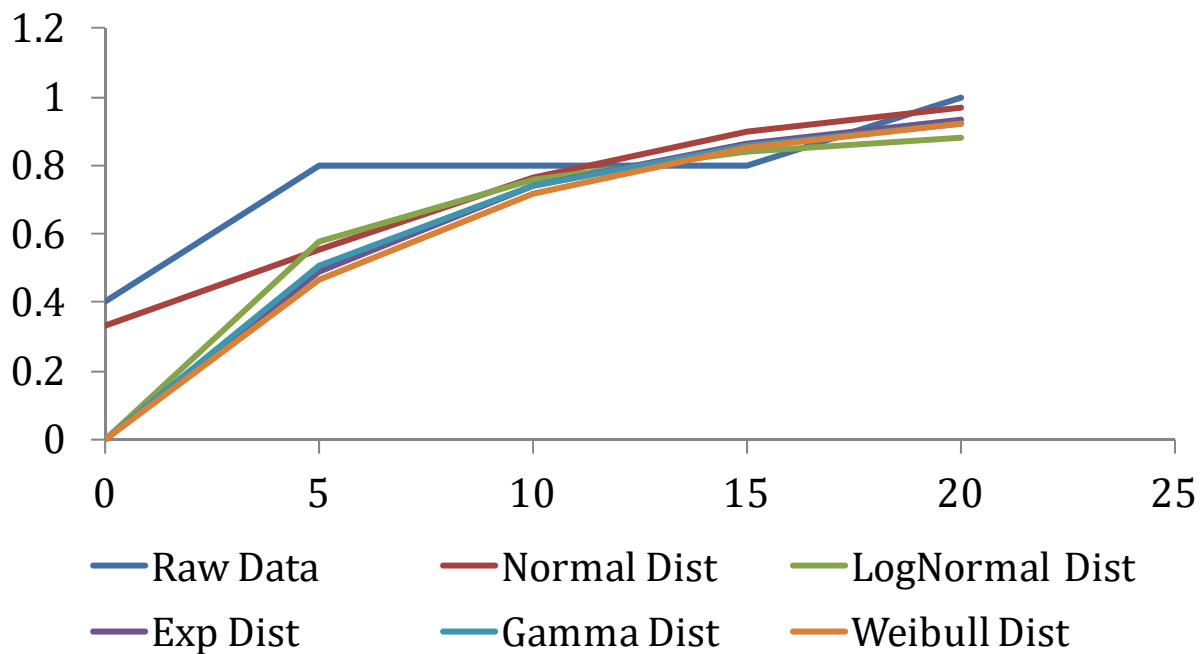


Figure 89: Cumulative Probability Functions, CO End, Multivariate/Tankless Water Heaters

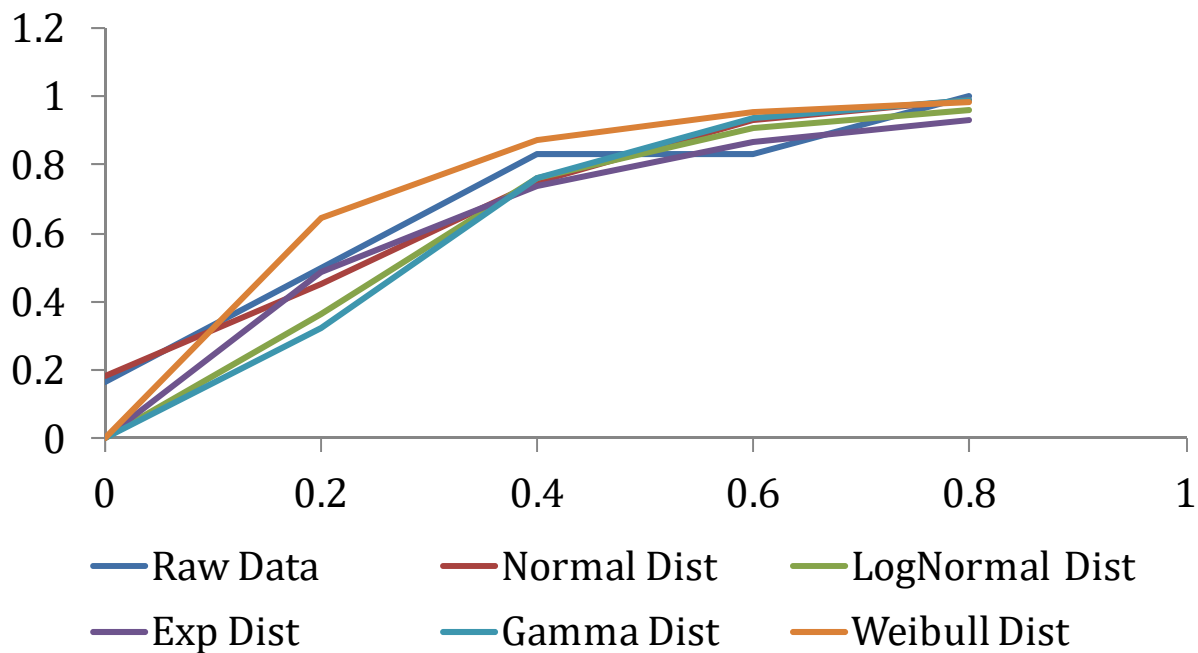


Figure 90: Cumulative Probability Functions, NO₂, Multivariate/Tankless Water Heaters

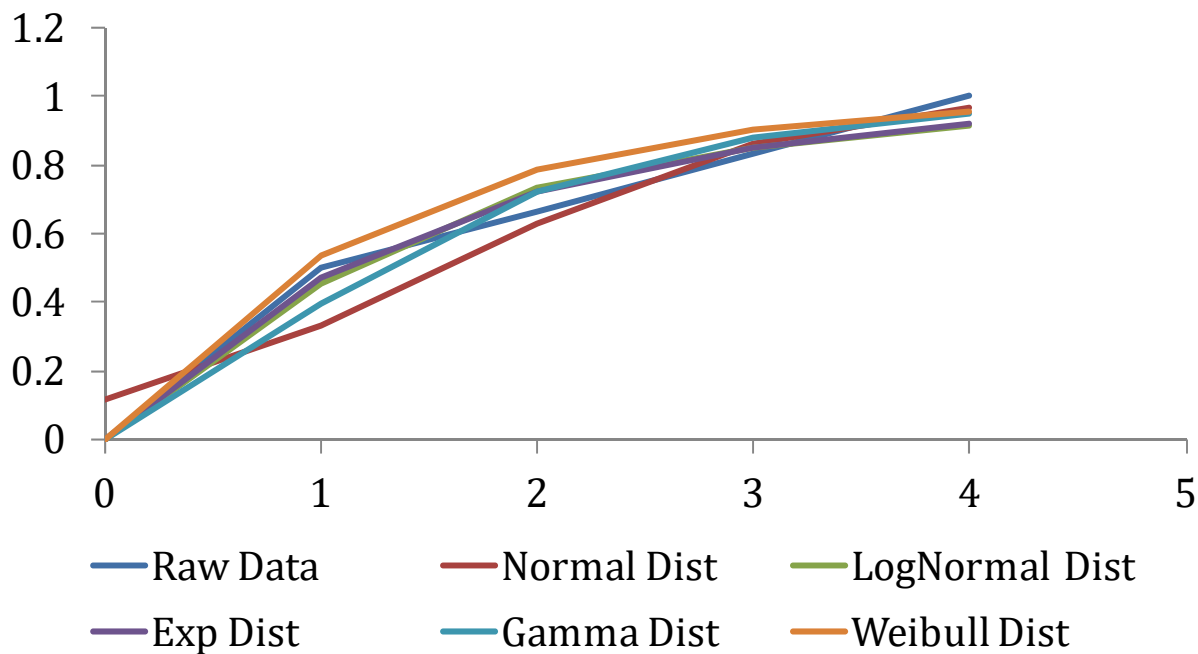


Figure 91: Cumulative Probability Functions NO_x, Multivariate/Tankless Water Heaters

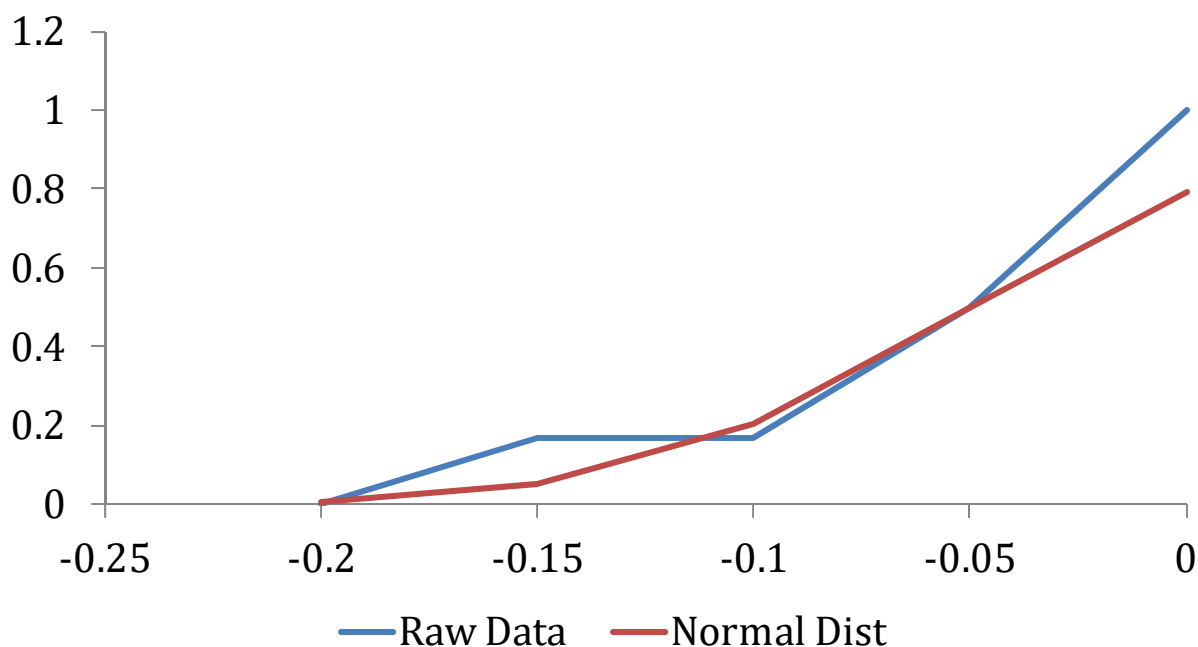


Figure 92: Cumulative Probability Functions, HCHO, Bivariate/Tankless Water Heaters

XXII.E Reliability Tables

The columns in the following tables represent the various point requirements as described in Section XVIII.D. The first five columns thus represent the assessment of the Sample Data Reliability; the last five columns assess the Distribution Reliability. The sum of a given row corresponds to the total reliability score previously provided in boxplots.

Table 31: Reliability Scores, Cooktops

	n≥5	n≥10	p≤0.1	R2≥0.75	p&R2	AD≤0.35	p≥0.75	R2≥0.8	Round 1	Round 2
CO, Full	1	1	1	1	1	1	1	1	0	0
CO, End	1	1	1	1	1	1	1	1	2	-
NO2 Full, No Outlier	1	1	0	0	0	0	0	1	0	1
NO2 End, No Outlier	1	1	0	0	0	0	0	0	0	0
HCHO, No Outlier	1	0	0	0	0	0	0	0	0	0
NOX, Full	1	1	0	0	0	0	0	1	0	1
NOX, End	1	1	1	0	1	1	1	1	0	1

Table 32: Reliability Scores, Broilers

	n≥5	n≥10	p≤0.1	R2≥0.75	p&R2	AD≤0.35	p≥0.75	R2≥0.8	Round 1	Round 2
CO, Full	1	0	1	1	1	1	0	1	2	-
CO, End	1	0	1	0	1	0	0	0	2	-
NO2, Full	1	0	1	0	0	1	1	1	2	-
HCHO	0	0	0	1	0	1	1	1	2	-
NOX, Full	1	0	1	0	0	1	0	1	0	0

Table 33: Reliability Scores, Ovens

	n≥5	n≥10	p≤0.1	R2≥0.75	p&R2	AD≤0.35	p≥0.75	R2≥0.8	Round 1	Round 2
CO, Bi	1	1	1	0	0	0	0	1	2	-
NO2, Bi	1	1	0	0	1	1	1	1	2	-
HCHO, Bi	1	1	0	0	1	0	0	0	0	0
CO, Multi	1	1	1	1	1	0	0	1	2	-
NO2, Multi	1	1	1	1	1	1	1	1	2	-
NOX, Multi	1	1	0	1	1	1	1	1	2	-

Table 34: Reliability Scores, Furnaces

	n≥5	n≥10	p≤0.1	R2≥0.75	p&R2	AD≤0.35	p≥0.75	R2≥0.8	Round 1	Round 2
CO, Full	1	0	1	1	1	1	1	1	2	-
CO, End	1	0	1	1	0	0	0	0	2	-
NO2, Full	1	0	0	0	0	0	0	0	0	0
HCHO	0	0	1	1	1	0	0	0	0	0
NOX	1	0	1	1	1	0	0	1	2	-

Table 35: Reliability Scores, Storage Water Heaters

	n≥5	n≥10	p≤0.1	R2≥0.75	p&R2	AD≤0.35	p≥0.75	R2≥0.8	Round 1	Round 2
CO	1	0	1	1	1	0	0	0	0	0
NO2	1	0	1	1	1	1	1	1	2	-
NOX	1	0	1	0	0	0	0	0	0	0

Table 36: Reliability Scores, Tankless Water Heaters

	n≥5	n≥10	p≤0.1	R2≥0.75	p&R2	AD≤0.35	p≥0.75	R2≥0.8	Round 1	Round 2
HCHO, Bi	1	0	0	1	1	0	0	1	2	-
CO Full, Multi No Outlier	1	0	1	1	1	0	0	0	0	0
CO End, Multi No Outlier	1	0	1	1	1	0	0	0	0	0
NO2 Multi	1	0	1	1	1	1	0	0	0	0
NOX, Multi	1	0	1	1	1	1	1	1	0	0

