A Quantitative Analysis of the Uncertainty of Emissions Data - A Limited Study

William B. Kuykendal, EPA/OAQPS; Jennifer Filipowski, North Carolina State University Intern; Thomas B. McMullen, Senior Environmental Employee

Abstract

The emission inventory community has long struggled with the issue of the uncertainty of emissions estimates and how to quantify it. The basic difficulty is that for the most part there is not a known standard value of emissions data against which various estimates of emissions can be evaluated for uncertainty. This paper presents an analysis of the robust continuous emissions monitoring (CEM) utility data base from Southern Company Services and compares these data with emissions estimates that are made using AP-42 emission factors. We posit that the quality assured CEM data approach the true value. The emission factor derived emission estimates are then compared to the CEM emissions. The analysis examined SO_2 and NO_X data for multiple source classification codes (SCC) both with and without emission control devices and shows results of variation within groupings of sources by SCCs and by individual sources. The analysis also evaluates whether or not there is bias in the emission factor derived estimates.

Introduction

The uncertainty of emissions data and how to estimate and quantify it, has been identified by the NARSTO emission inventory assessment[1] as one of the major needs for improving an emission inventory program. The purpose of this paper is to quantify, in a limited way, the uncertainty of emission factor derived emission estimates as compared with continuous emission monitoring (CEM) emission estimates. The paper assumes that that the CEM derived estimates are closer to the true value of emissions than the emission factor values. While there are uncertainties associated with the CEM data, for example, the sampling system and the CEM analyzer each have uncertainties associated with them, most emission inventory practitioners would agree with this assumption. The NARSTO emission inventory assessment also states this as a given.

The approach was to mimic what an air pollution control agency might do to estimate emissions from certain point sources if these sources did not have CEM data. Emission factors were obtained from AP-42[2] for the relevant source categories and used to calculate the individual source emissions. These emission factor based emission estimates were then compared to the CEM derived emission estimates.

In order to implement this approach, it was necessary to locate a suitable database of CEM based emissions data. Southern Company Services, Inc., presented a paper at the 2005 emission inventory conference[3] that described the development of a database that used CEM data to estimate hourly emissions to support regional haze modeling. Southern Company graciously agreed to share this database with EPA for the purpose of this evaluation.

Development of the Database

The database as received from Southern Company was an Excel spreadsheet that contained hourly emissions data for sulfur dioxide (SO_2), oxides of nitrogen (NO_X), carbon monoxide (CO), volatile organic compounds (VOCs), and total filterable particulate matter for each electric generating unit in the Southern Company system for the year 2002. In order to perform the comparative analysis between the CEM emission estimates and emission factor based estimates, several additions were made to the database. These changes are summarized as follows.

- Hourly emission estimates were too fine a temporal resolution for this study; the hourly data were rolled up to monthly CEM based estimates.
- In order to select the appropriate AP-42 emission factor, additional information on emission control technology needed to be added on a unit by unit basis.
- Based on the combination of source category type (source classification code – SCC) and emission control technology, an appropriate emission factor was selected from AP-42. The basic emission estimation equation from AP-42 was used.

$$E = A \times EF \times (1 - ER / 100) \quad \text{(Equation 1)}^2$$

Where:

E = Emissions
A = Activity Rate
EF = Emission Factor
ER = Overall Emission Reduction Efficiency, %

- The original spreadsheet included all of the electric generating units in the Southern Company system. However, only the coal fired units had CEMs in substantial numbers. Therefore, it was decided to limit the comparison to these units.
- To apply the emission factor, fuel burned needed to be added. The heat input was known for each unit by month. This was used with the heating value of the coal to calculate the mass of fuel burned. To estimate SO_2 emissions, the fuel sulfur content was added to the spreadsheet.
- While the original spreadsheet included emissions for SO_2, NO_X, CO, VOC and particulate matter, only the SO_2 and NO_X emissions were derived from CEM data. Therefore, the comparison with the emission factor data was limited to these two pollutants and only SO_2 and NO_X were included in the final database.

The completed data base consisted of a total of 67 units and is summarized in Table 1. Five basic types of steam generator combustors are represented with the majority being either tangentially fired or wall fired bituminous coal units. The range of emission factors selected is included in Table 1. Also in this table is the overall emission reduction efficiency range. Overall emission reduction efficiency range as used in this paper, is a term that includes any adjustment to the basic emission factor used to calculate emissions in the above equation. This term includes the control efficiency of any control device present.

Table 1

Combustor Type	Emission Factor Range		Emissions Reduction Efficiency Range		Number of Units
	NO_x	SO_2	NO_x	SO_2	
Tangentially Fired Bituminous	**9.7-15**	**38S**	**0-78.5**	**0-92.5**	**36**
Wall Fired Bituminous	**11-22**	**38S**	**0-78.5**	**0**	**19**
Cell Burner Bituminous	**31**	**38S**	**45**	**0**	**4**
Tangentially Fired Sub-bituminous	**7.2**	**35S**	**17.5**	**0**	**4**
Wall Fired Sub-bituminous	**7.4**	**35S**	**0**	**0**	**4**
TOTAL					**67**

Analysis of the Data

The analytical approach was to compare the CEM measured data with the corresponding AP-42 emission factor calculated emissions to gain some insight in to the uncertainty of the emission factor method. Comparisons were made to evaluate the following:

- Was there a pattern of variability in the two methods on a temporal basis?
- Were there significant differences attributable to combustor type, burner configuration or control techniques?
- Were there significant differences in the situations when the overall emission reduction efficiency term was applied versus when this term was not used?

Most of the analysis looked at the NO_X data because there were a variety of NO_X controls used on the 67 units. Only one unit in the database had SO_2 controls.

Results

Figures 1(a), 1(b), and 1(c) show monthly NO_X emissions data for the CEMs and AP-42 for three representative combustor types and burner configurations. The figures show that the AP-42 results track the CEM data very closely. Where a bias is present (Figures 1(a) and 1(c)), it is small and consistent. Figure 1(b) shows data from 3 units that use Secondary Catalytic Reduction (SCR) NO_X control technology. The SCR's only operate during the five month ozone season. During the remaining seven months, these units operate as low NO_X burner units. Note that when operating in the SCR mode, the CEM data shows that the first and last months of operation (May and September) have higher emissions indicating that there is a "ramp up" and "ramp down" associated with the process that is not captured by the AP-42 method. Overall, these results demonstrate that there is not any temporal variability between the CEM data and the AP-42 emission estimates.

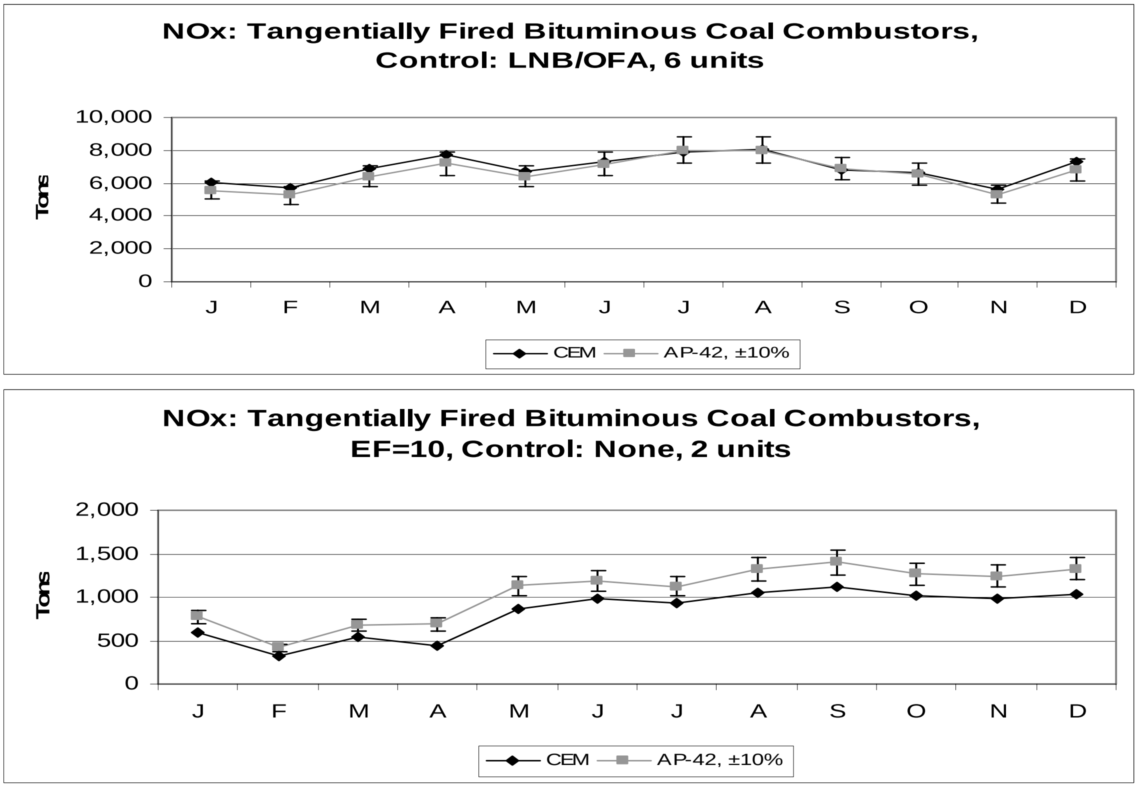


Figure 1(a)

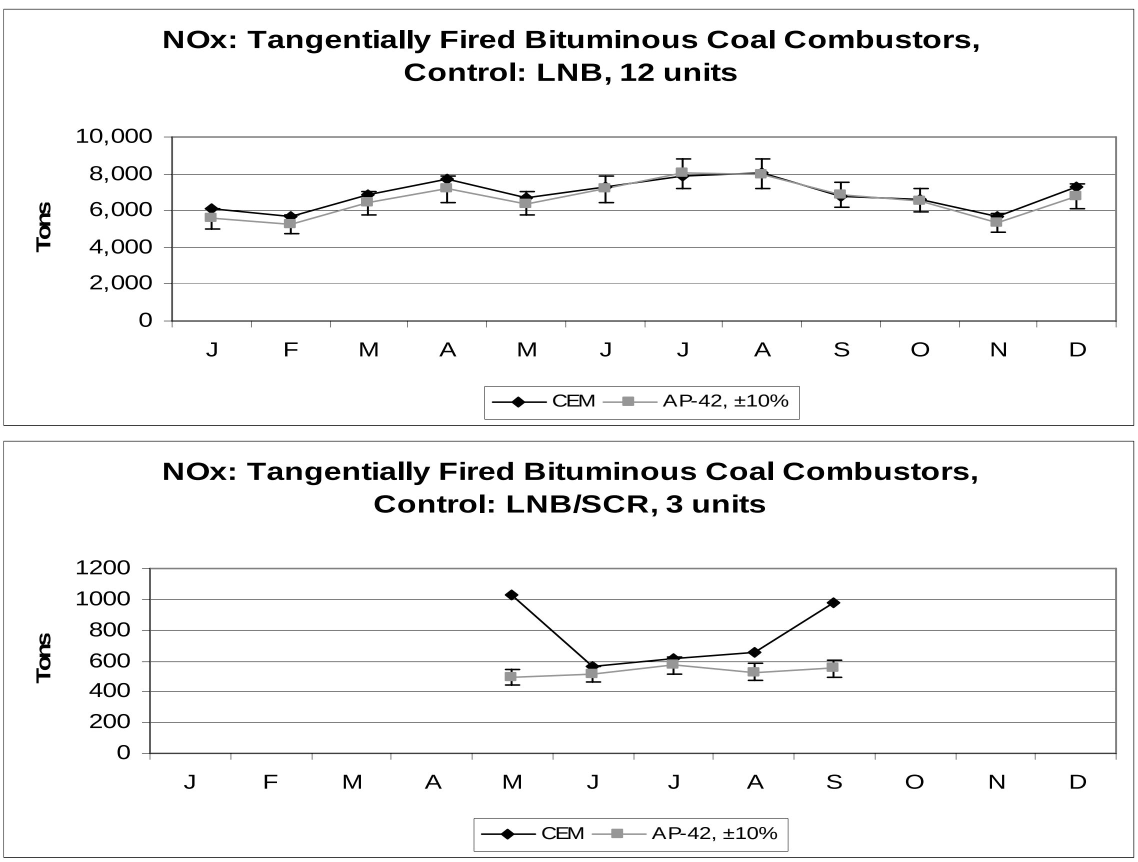


Figure 1(b)

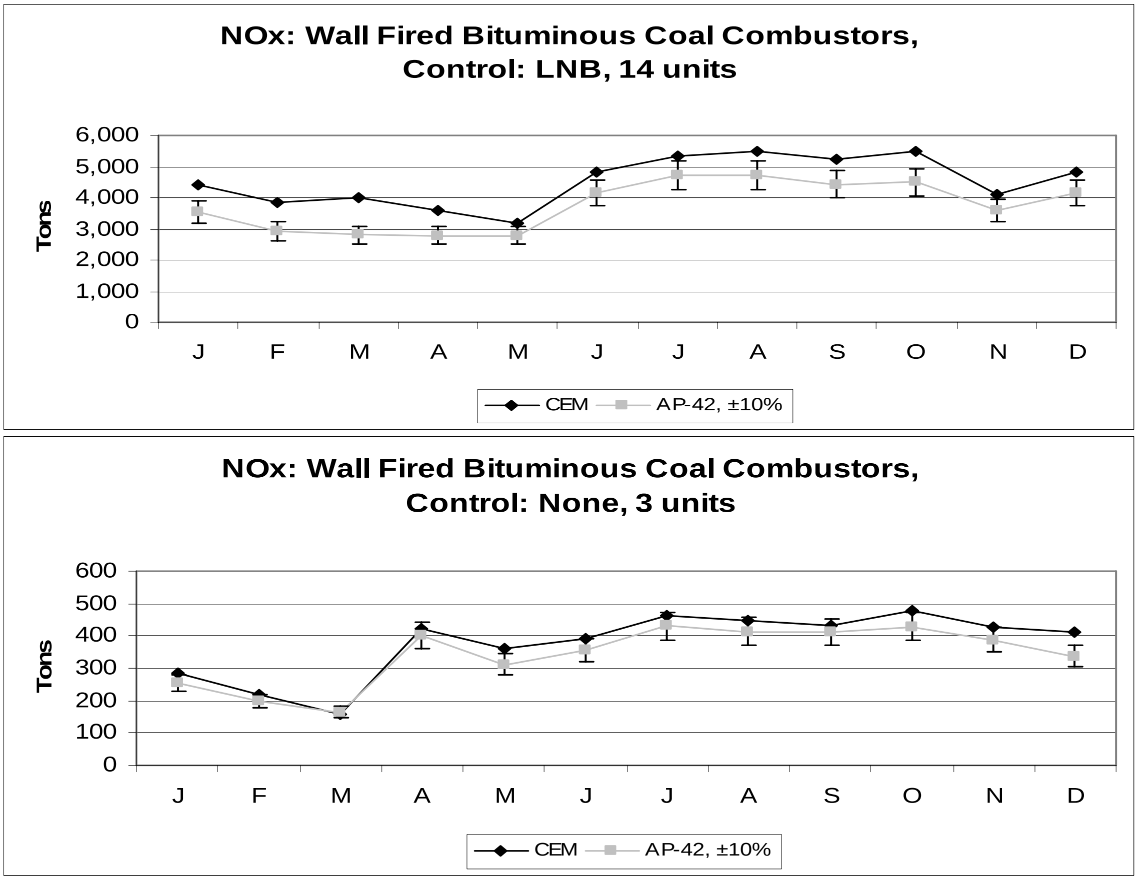


Figure 1(c)

Figures 2 – 7 show the variability of the "implied emission factor" for several different combustor type/emission control combinations. "Implied emission factor" is the emission factor calculated from the monthly CEM emission measured data. These histograms give a sense of the variability of the emission factor data and how it compares to the AP-42 emission factor. For example, Figure 3 looks to be a normally distributed range of "implied emission factors" with a central value of 14. This compares favorably with the AP-42 emission factor of 15. Figure 7 has a bimodal distribution. The newer units, from 1960 and later, are in reasonable agreement with the AP-42 value of 11. The older units, 1955 and older, show significantly higher emissions than would be predicted from the AP-42 emission factor.

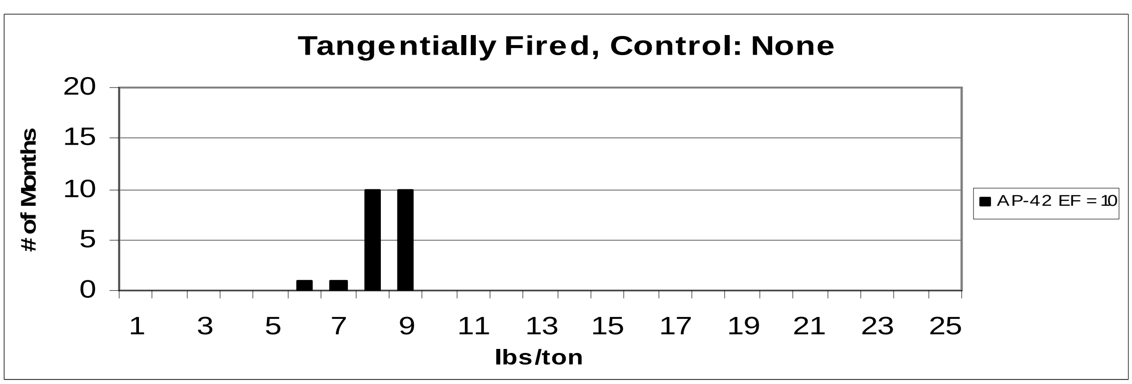


Figure 2

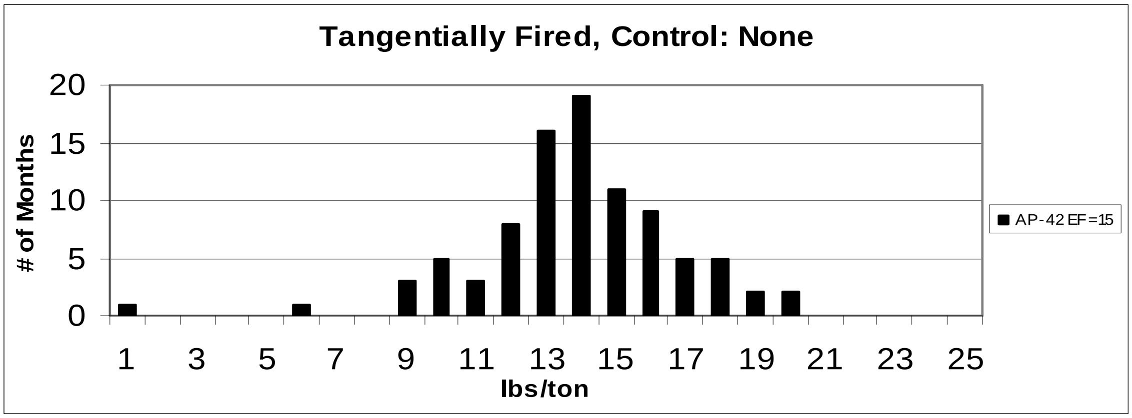


Figure 3

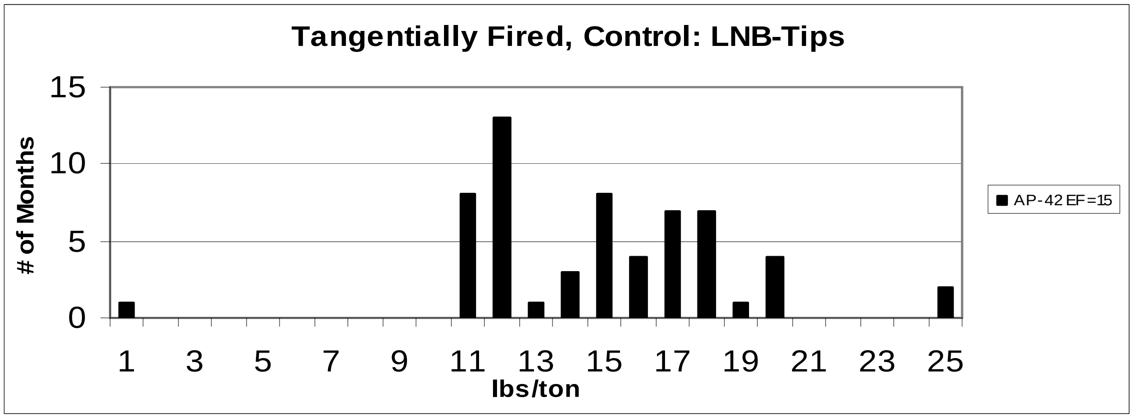


Figure 4

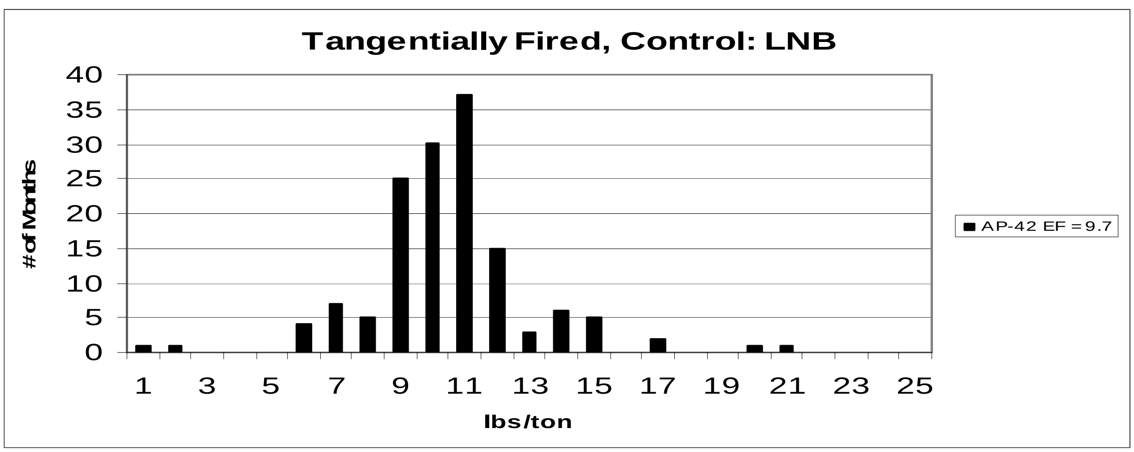


Figure 5

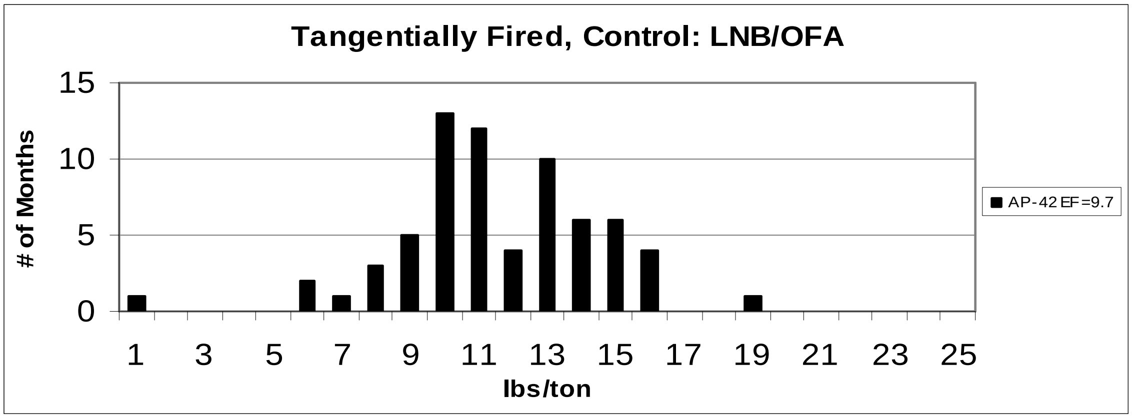


Figure 6

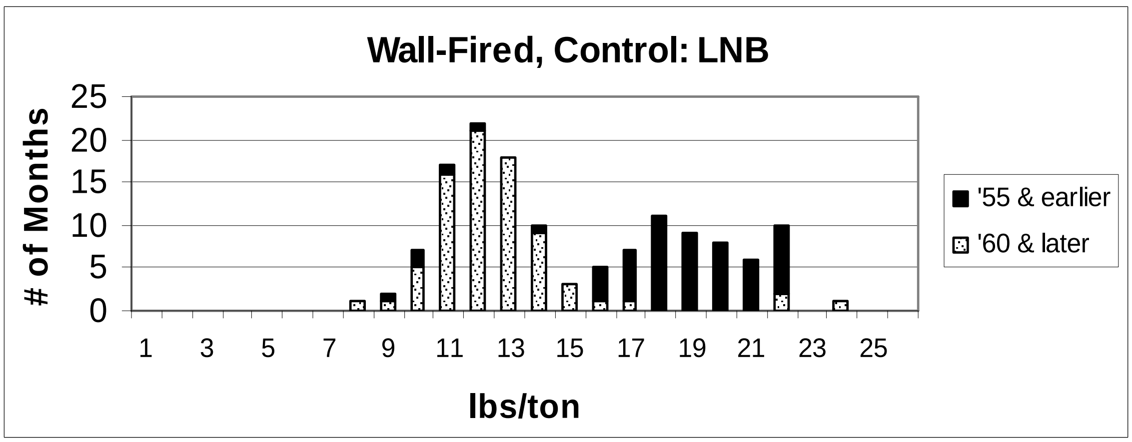


Figure 7

Because there were a significant number of both tangentially fired and wall fired bituminous coal units, analysis was done to look at the effects of various burner configurations and control technologies. Figures 8 – 12 show the results for the 36 tangentially fired bituminous coal units in the study. The results for the 10 units with no NO_X controls are shown in Figure 8. The NO_X results are well correlated, but show positive bias for the AP-42 estimates. The SO_2 results have excellent overall agreement, a trend that holds true for all of the results that follow. This is understandable because the SO_2 factor is based on a material balance approach and with only one exception, there are no SO_2 controls. The results for the 5 units with “low NO_X burner tips” are shown in Figure 9. The NO_X results exhibit more scatter, but the agreement is still good. The largest number of units in the study, 12, used “low NO_X burners” for NO_X control. These results are shown in Figure 10. Again, agreement is good for both NO_X and SO_2. The only unit in the study with SO_2 controls is in this group. This unit has a limestone scrubber with forced oxidation to control SO_2. In the case of this unit, a range of control efficiency of 90 – 95% was given by the utility. The AP-42 estimate assumed a control efficiency of 92.5%. Based on the CEM data, the actual efficiency was 95%. Nevertheless, the overall agreement between the AP-42 SO_2 estimate and the CEM measurement continued to be excellent. Figure 11 shows the results for the 3 units in the study that used low NO_X burners coupled with secondary catalytic reduction for enhanced NO_X control. The secondary catalytic reduction was only operated during the five month May – September ozone season. During the five months when the secondary catalytic reduction process was in operation, the AP-42 estimates under predicted

NO_X emissions by about 30%, primarily caused by the "ramp-up" and "ramp-down" phenomenon noted in the discussion on Figure 1(b). The results for the six units equipped with low NO_X burners coupled with over fire air are shown in Figure 12.

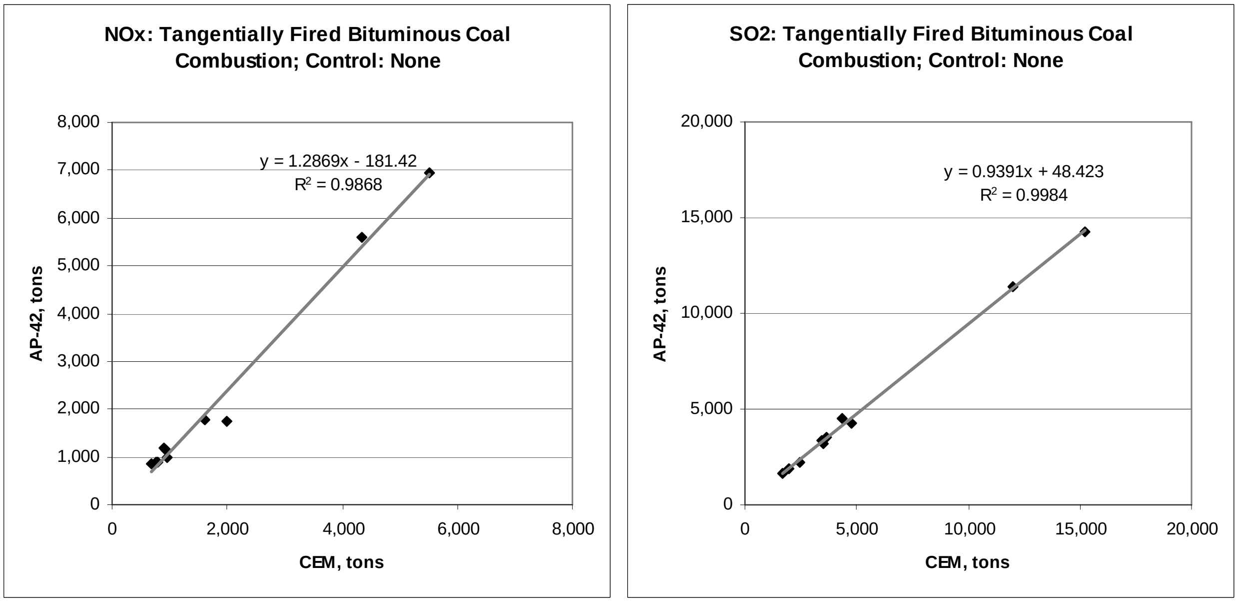


Figure 8

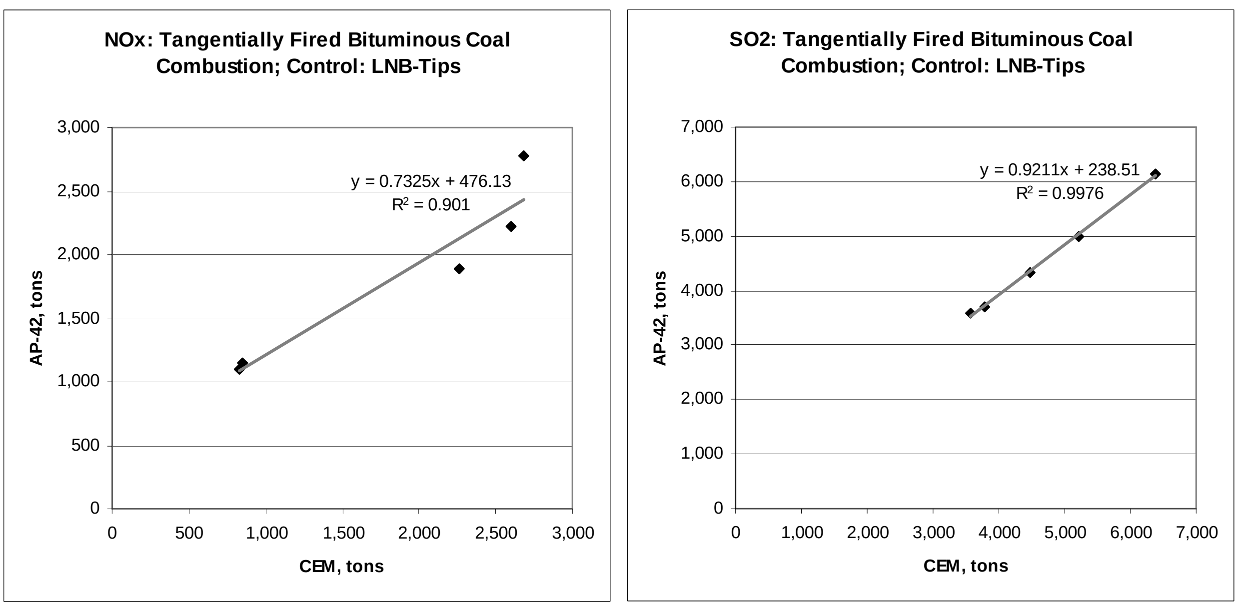


Figure 9

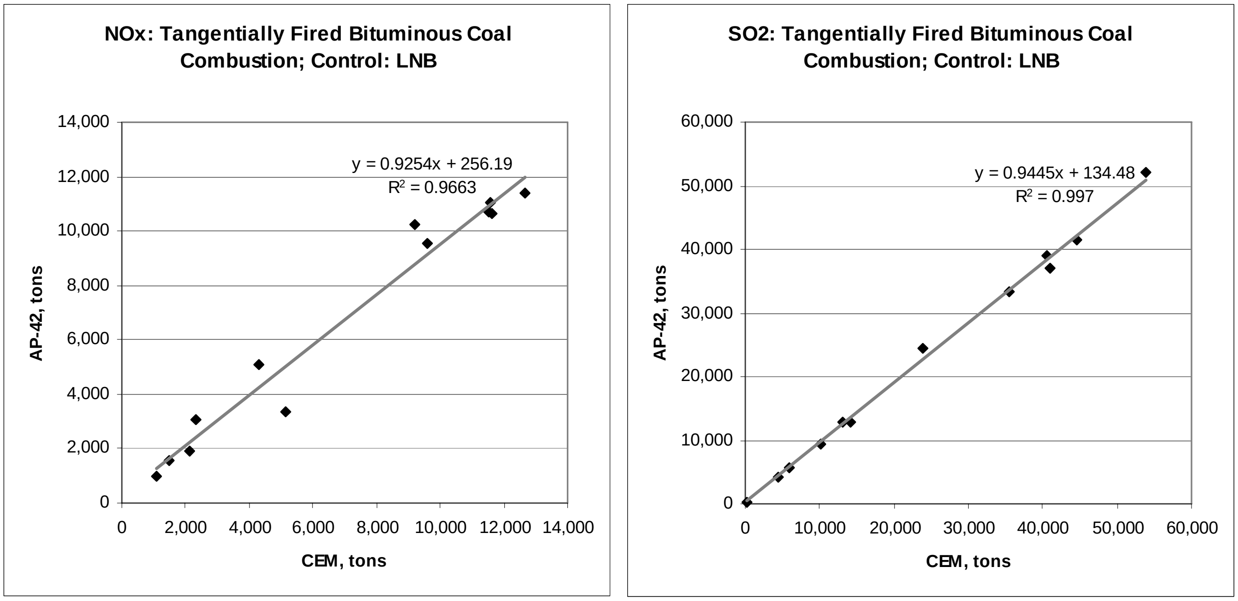


Figure 10

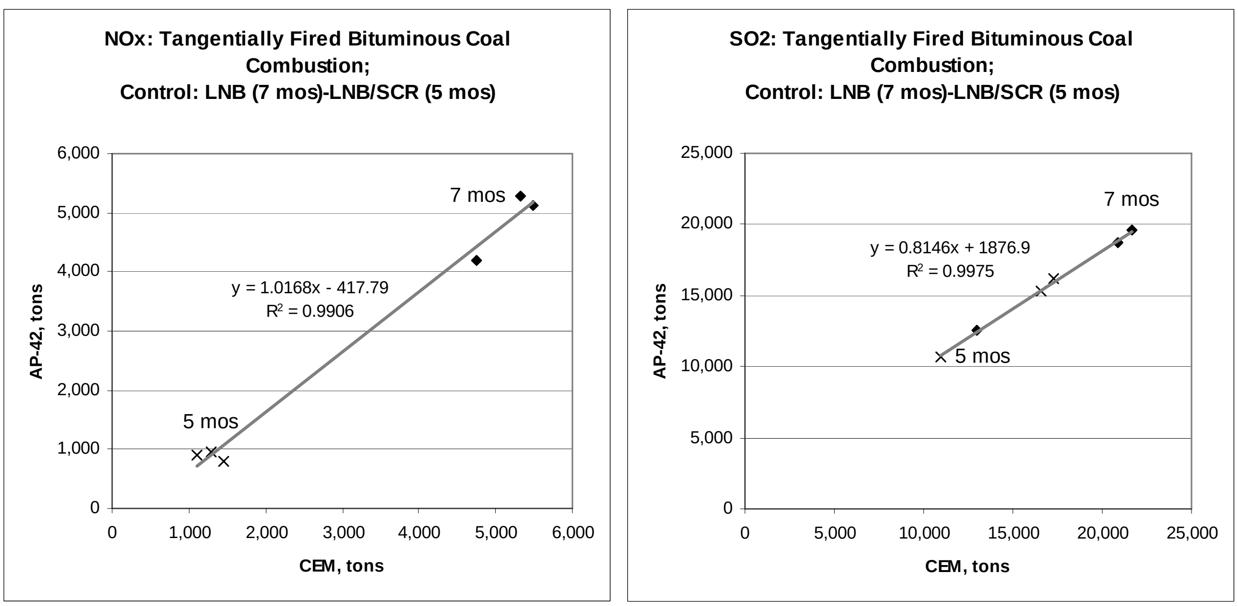


Figure 11

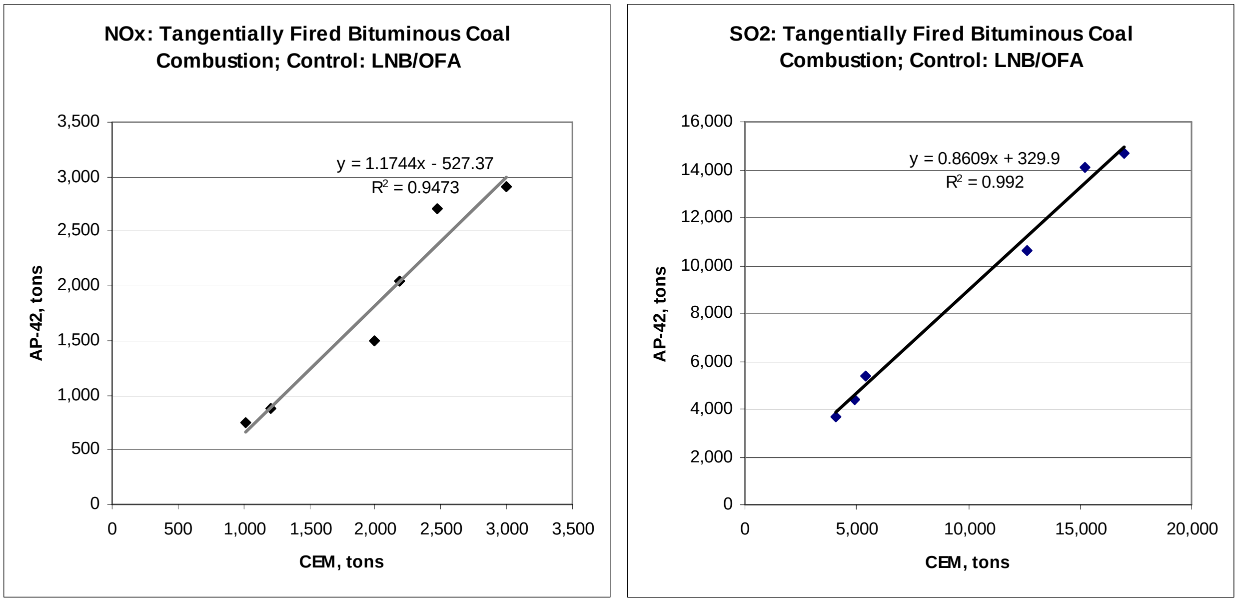


Figure 12

The results for all 36 tangentially fired bituminous units are presented in Table 2. Note that the NO_X results, while exhibiting more scatter, have both positive and negative bias which tend to offset giving an overall agreement of about 2%. For SO_2, the AP-42 results consistently under predict the CEM measurements averaging 6%.

Table 2

Units	Control Eq	Tangentially Fired Bituminous Coal Combustors	AP-42 NOx (tons)	CEM NOx (tons)	% Difference	AP-42 SO2 (tons)	CEM SO2 (tons)	% Difference
10	None	**SUM:**	**21,995**	**18,501**	**-18.88%**	***50,249***	***52,992***	***5.18%***
		MAX:	6,947	5,512	13.01%	*14,273*	*15,213*	*10.37%*
		MIN:	841	673	-32.34%	*1,667*	*1,653*	*-3.65%*
5	LNB Tips	**SUM:**	**9,141**	**9,228**	**0.95%**	**22,765**	**23,421**	**2.80%**
		MAX:	2,780	2,678	16.31%	6,151	6,377	4.23%
		MIN:	1,103	834	-34.63%	3,591	3,565	-0.75%
12	LNB	**SUM:**	**79,594**	**82,691**	**3.75%**	**272,894**	**287,208**	**4.98%**
		MAX:	11,394	12,678	34.42%	52,208	53,783	9.44%
		MIN:	980	1,091	-31.68%	303	263	-15.13%
3	*LNB, 7 mos*	***SUM:***	***14,579***	***15,584***	***6.45%***	***50,872***	***55,503***	***8.3%***
		MAX:	*5,274*	*5,497*	*11.97%*	*19,570*	*21,660*	*10.4%*
		MIN:	*4,185*	*4,754*	*1.10%*	*12,609*	*12,984*	*2.9%*
15	LNB, All	**SUM:**	**94,172**	**98,275**	**4.17%**	**323,766**	**342,711**	**5.53%**
		MAX:	11,394	12,678	34.42%	52,208	53,783	10.4%
		MIN:	980	1,091	-31.68%	303	263	-15.13%
3	LNB/SCR. 5 mos	**SUM:**	**2,665**	**3,841**	**30.61%**	**42,148**	**44,862**	**6.0%**
		MAX:	955	1,444	44.15%	16,182	17,273	7.83%
		MIN:	807	1,113	18.82%	10,661	10,982	2.92%
6	LNB/OFA	**SUM:**	**10,783**	**11,876**	**9.20%**	**52,919**	**59,173**	**10.57%**
		MAX:	2,907	2,998	27.34%	14,706	16,951	15.74%
		MIN:	743	1,011	-9.43%	3,698	4,076	0.02%
36		**GRAND SUM:**	**138,757**	**141,721**	**2.09%**	**491,847**	**523,159**	**5.99%**
		MAX:	11,394	12,678	44.15%	52,208	53,783	15.74%
		MIN:	743	673	-34.63%	303	263	-15.13%

Results for the 19 wall fired bituminous coal units are shown in Figures 13 and 14 and summarized in Table 3. In the case of the NO_X results, there is a bias, with the AP-42 emissions underestimating the CEM measurement on average by about 17%. As with the tangential units, the SO_2 results on average agree within about 6%, also under predicting the measured results.

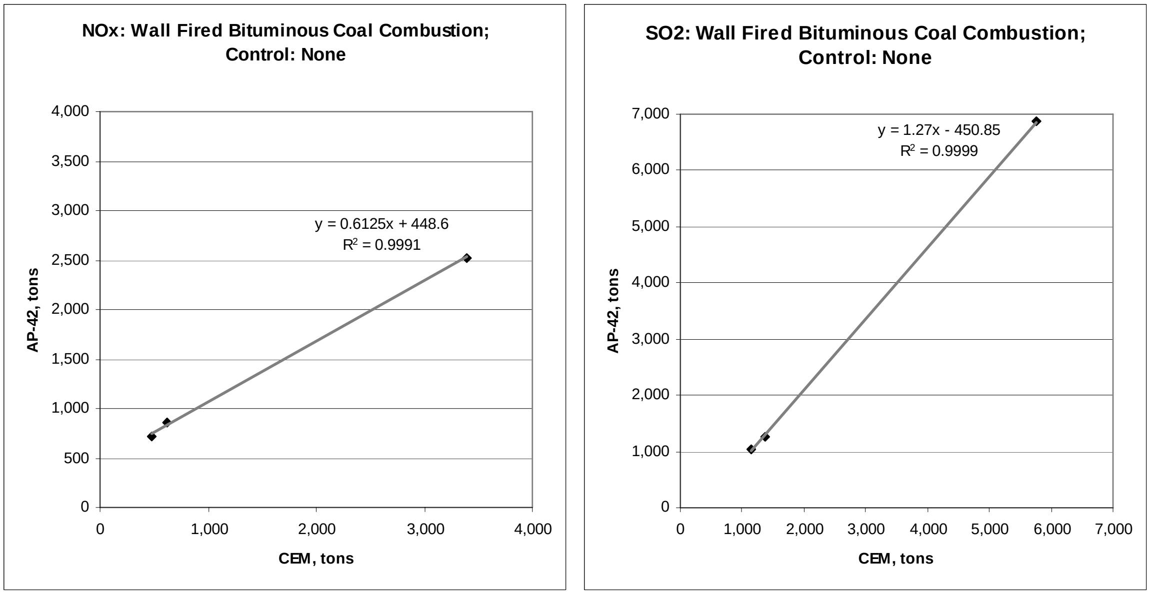


Figure 13

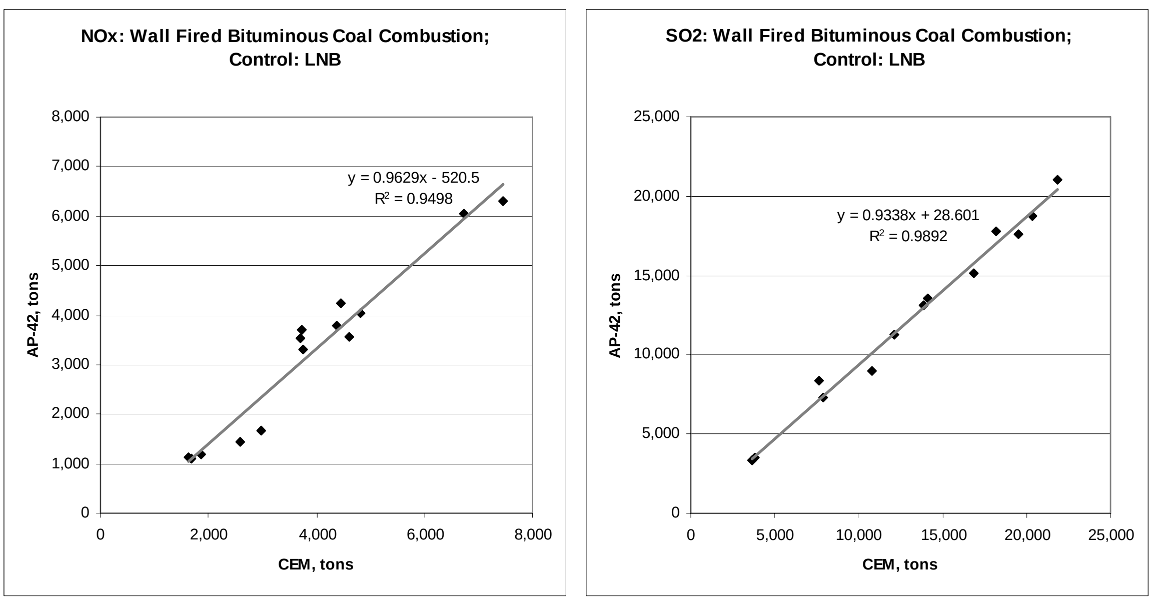


Figure 14

Table 3

Units	Control Eq	Wall Fired Bituminous Coal Combustors	AP-42 NOx, tons	CEM NOx, tons	% Diff.	AP-42 SO_2, tons	CEM SO_2, tons	% Diff.
3	None	**SUM:**	**4,095**	**4,489**	**8.77%**	**9,164**	**8,281**	**-10.67%**
		MAX:	2,528	3,397	25.59%	6,864	5,759	10.06%
		MIN:	712	478	-49.04%	1,037	1,153	-19.19%
14	LNB	**SUM:**	**45,054**	**54,355**	**17.11%**	**163,139**	**174,266**	**6.39%**
		MAX:	6,291	7,451	44.17%	21,011	21,810	16.79%
		MIN:	1,107	1,619	0.77%	3,315	3,622	-10.23%
1	LNB/OFA		2,853	3,986	28.42%	14,728	15,532	5.18%
1	LNB/OFA, 7 mos		2,082	2,568	18.94%	15,870	17,044	6.89%
	LNB/OFA/SCR, 5 mos		501	724				
19		**GRAND SUM:**	**54,084**	**65,398**	**17.30%**	**202,901**	**215,123**	**5.68%**
		MAX:	6,291	7,451	44.17%	21,011	21,810	16.79%
		MIN:	1,107	1,619	0.77%	3,315	3,622	-10.23%

Figures 15 – 17 show the results for three groups of four units each with differing combustor types, coal and no specified controls for NO_X or SO_2. As with the tangential and wall fired units, the agreement is good for SO_2. However, in the case of NO_X, the agreement is not good in two of the three cases, differing by as much as 49%. As seen in Figures 15 and 17, the NO_X results are clustered by individual unit indicating that there are unit specific characteristics that influence NO_X emissions that are not captured in the assigned AP-42 NO_X emission factor.

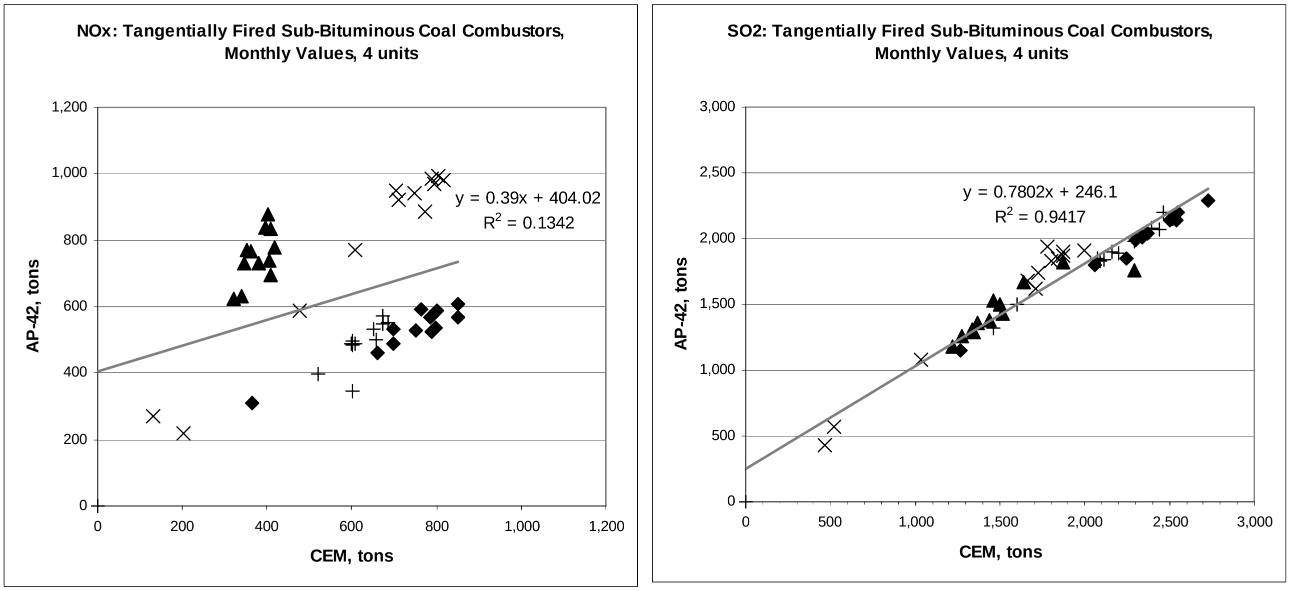


Figure 15

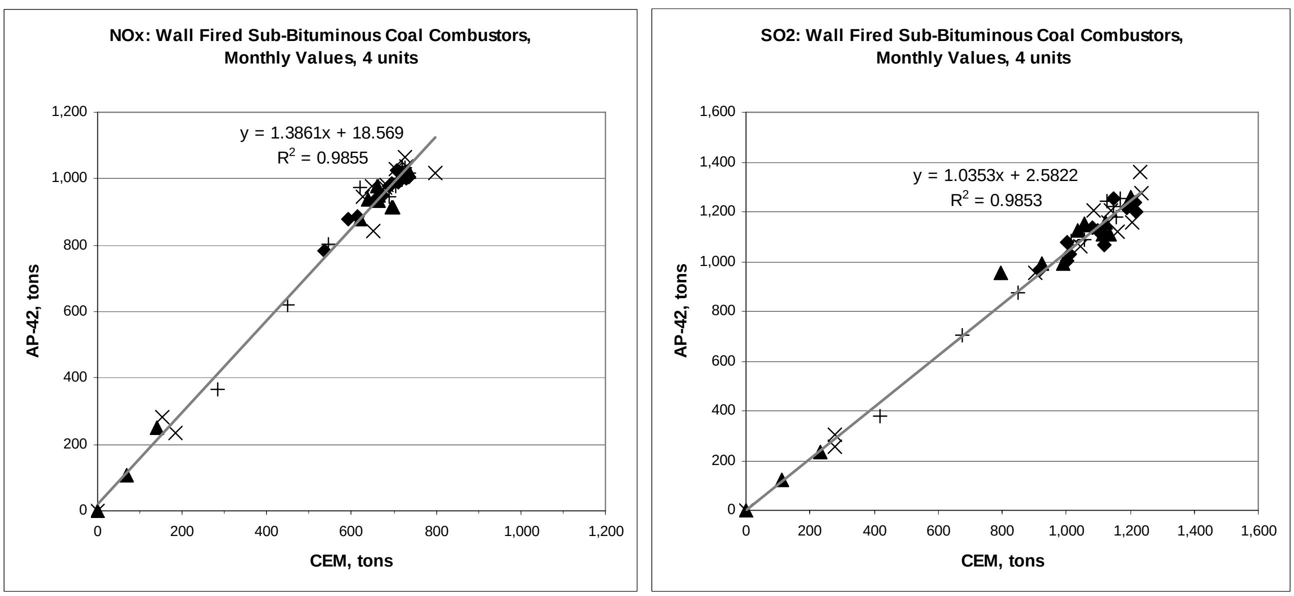


Figure 16

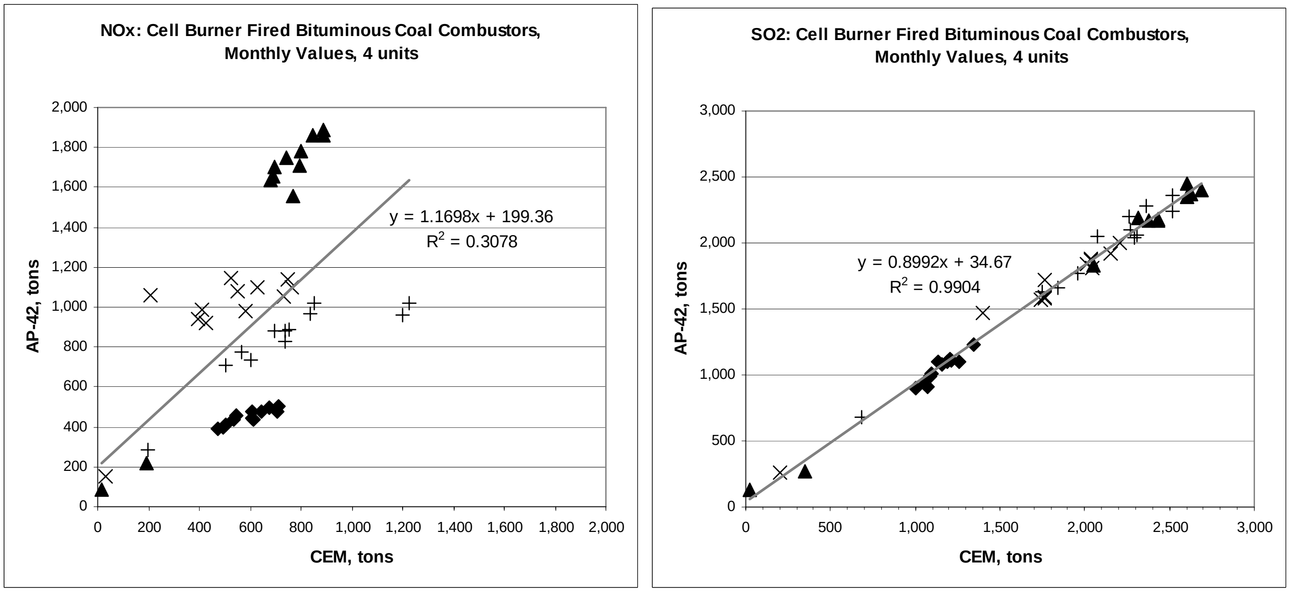
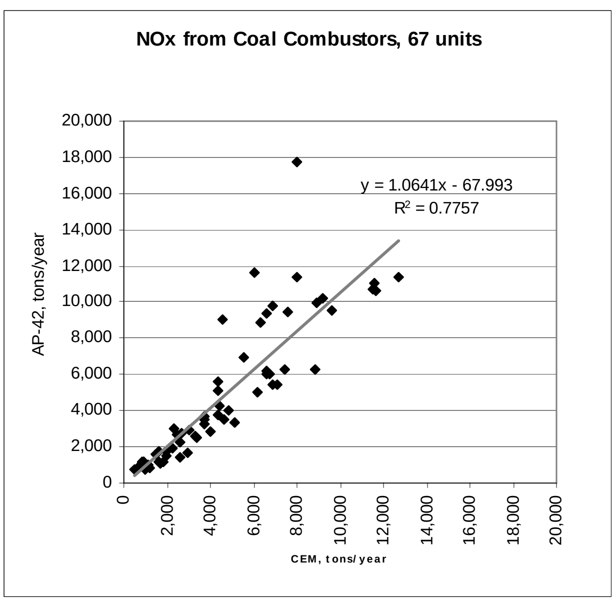


Figure 17

All of the results for the 67 units are summarized in Figure 18. These overall results show that the AP-42 estimates for both NO_X and SO_2 agree in the range of 5%. For NO_X, the results show significantly more variability, with the average showing that the AP-42 estimates over-predicts emissions. The SO_2 results are highly correlated with little variability. The AP-42 SO_2 estimate under-predicts the measured emissions.

NOx COAL	Units	Emission Factor NOx (tons)	CEM NOx (tons)	% Difference
Wall Fired Bituminous Coal Combustors	19	54,585	66,122	17.45%
Tangentially Fired Bituminous Coal Combustors	36	138,757	141,721	2.09%
Cell Burner Fired Bituminous Coal Combustors	4	44,699	30,031	-48.84%
Wall Fired Sub-Bituminous Coal Combustors	4	39,464	27,828	-41.81%
Tangentially Fired Sub-Bituminous Coal Combustors	4	30,225	27,775	-8.82%
	67	**307,730**	**293,478**	**-4.86%**

SO2 COAL	Units	Emission Factor SO2 (tons)	CEM SO2 (tons)	% Difference
Wall Fired Bituminous Coal Combustors	19	202,901	215,123	5.68%
Tangentially Fired Bituminous Coal Combustors	36	495,581	523,159	5.27%
Cell Burner Fired Bituminous Coal Combustors	4	78,043	84,937	8.12%
Wall Fired Sub-Bituminous Coal Combustors	4	45,902	44,218	-3.81%
Tangentially Fired Sub-Bituminous Coal Combustors	4	80,162	87,609	8.50%
	67	**902,588**	**955,047**	**5.49%**



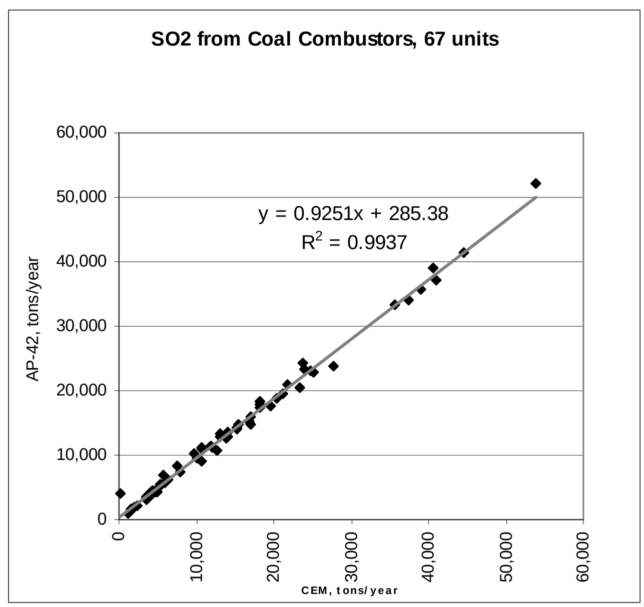


Figure 18

The above analysis focused on the influence of the various parameters such as combustor type, fuel, and type of emission controls as they relate to the selection and application of an emission factor. While this analysis might prove useful in further improving the respective emission factors, the purpose of this analysis was to evaluate the uncertainty of the emission estimation process. One additional analysis was done to determine if the estimation method itself could account for some of the uncertainty. The approach was to evaluate whether or not the “overall emission reduction efficiency” term in Equation 1 could be associated with higher levels of uncertainty. The premise was that this term is an additive correction term to the basic emission factor, EF in Equation 1, and that there is likely to be additional uncertainty associated with the application of this term. The full database was divided in to two groups, one where the overall emission reduction efficiency term was used and the other where it was not. The results are shown in Figure 19. These results show that there is a significant degradation in the agreement between the AP-42 estimate and the CEM measurement when the overall emission reduction efficiency term is applied.

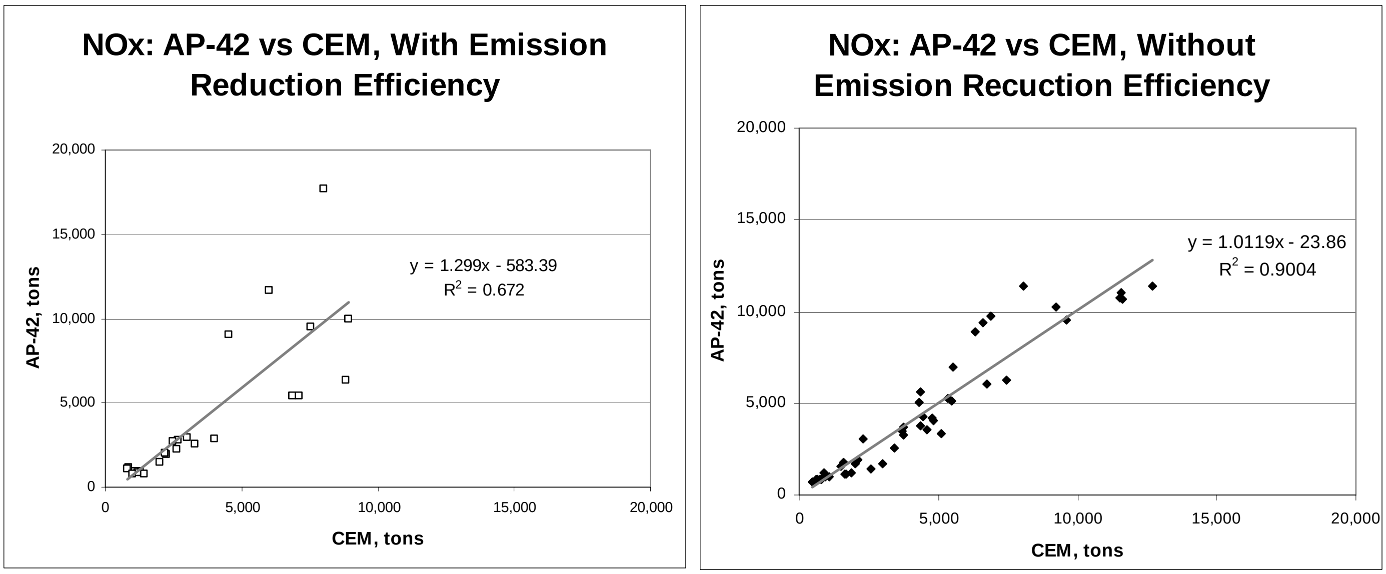


Figure 19

Conclusions and Discussion

The principle conclusion to be drawn from this analysis is that within the limits of the data, the application of high quality emission factors coupled with good activity data yields results that agree with measured data in the range of +/- 5%. Results for individual sources vary over a much wider range. In this study, the NO_X results had substantially greater variability than the SO_2 results for the same sources, but with no consistent bias. For SO_2, the results were very consistent with the AP-42 estimate being lower than the CEM measured values. The application of the “overall emission reduction efficiency” term was shown to be an additional source of uncertainty.

These results were presented at the 15th emission inventory conference in New Orleans in May 2006. As part of the presentation, after the development of the database and analytical approach were explained, but before the results were presented, the session attendees were asked to vote on how good they thought the agreement would be. The logic was that the attendees at the emission inventory conference had a level of expertise that would allow for an informed opinion. The results from this poll are presented below:

Percent Difference AP-42/CEM	Number of Votes
0 – 10	**1**
10 – 25	**10**
25 – 100	**16**
>**100**	**4**

These poll results, while not part of a designed study, are none the less informative. The results do illustrate that the general perception is that emission factor estimates have much higher uncertainty than the results of this study demonstrated.

Acknowledgement

The authors wish to thank Southern Company Services in general, and Krishnan Kandasamy and Fred Ellis in particular, for their cooperation in the development of the database used in this study.

---

[1] Improving Emission Inventories for Effective Air Quality Management Across North America – A NARSTO Assessment, NARSTO-05-001, 2005.
[2] AP 42, Fifth Edition, Compliation of Air Pollutant Emission Factors, Volume I: Stationary Point and Area Sources, http://www.epa.gov/ttn/chief/ap42/index.html
[3] Kandasamy, Ellis and Jansen, Developing Southern Company Emissions and Flue Gas Characteristics for VISTAS Regional Haze Modeling, 2005, http://www.epa.gov/ttn/chief/conference/ei14/session9/kandasamy.pdf