

**The Pros and Cons of Predictive, Parametric, and Alternative Emissions  
Monitoring Systems for Regulatory Compliance**

**Joseph J. Macak III**  
Mostardi Platt Environmental  
1520 Kensington Road, Suite 204  
Oak Brook, Illinois 60523-2139

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## INTRODUCTION

The promulgation of the New Source Performance Standards for Industrial-Commercial-Institutional Steam Generating Units (40 CFR 60, Subpart Db) in the 1980s set the stage for the use of predictive monitoring techniques (operations monitoring programs) as a method of demonstrating continuous emissions compliance. This was followed by the Clean Air Act Amendments of 1990, 40 CFR 75 Continuous Emissions Monitoring, and 40 CFR 64 Compliance Assurance Monitoring (proposed). These regulatory programs support the development and use of predictive, parametric, and alternative methods as a compliance assurance monitoring tool. Although continuous emissions monitoring (CEM) systems are generally considered the ultimate systems for compliance determinations next to reference method source testing, predictive, parametric, and alternative emissions monitoring systems have established an industry stronghold and gained regulatory support. Complete systems can be established for nitrogen oxides and sulfur dioxide, as well as carbon monoxide, volatile organic compounds, total hydrocarbons, and even particulate emissions.

This paper closely examines the pros and cons of using predictive, parametric, and alternative monitoring techniques for regulatory compliance. While many predictive and parametric monitoring systems are less expensive to install and operate than CEM systems, and demonstrate exceptional relative accuracy test results, this paper will provide the reader with a better understanding of the limitations of these systems.

## BACKGROUND

Predictive emissions monitoring (PEM) systems can be classified as a software-based continuous emissions monitoring (CEM) system in which key operating parameters are correlated to pollutant emission rates. A mathematical model is developed which then “predicts” emission levels based on the operating parameters. Approaches vary in developing a model that accurately predicts emissions from a source. Three common approaches to emission prediction models include the use of models based on: (1) first principles, (2) statistical regressions, and (3) artificial intelligence--neural networks or non-linear models.<sup>1</sup> Using high-order, non-linear regression techniques, “adaptive” models are trained using historic operating data, and are said to predict process behavior accurately and flexibly.<sup>2</sup>

The history of predictive emissions monitoring development goes back to the early 1970s when NO<sub>x</sub> emission mathematical models were undergoing development by gas turbine engineers from the Westinghouse Electric Corporation. The diffusion-limited-mixing model that was developed for a specific family of gas turbine can-type combustors demonstrated its capability to predict NO<sub>x</sub> emissions as influenced by changes in ambient conditions, operating conditions, combustor geometry, and the type of fuel used within the accuracy of the measurement techniques.<sup>3,4</sup>

The first reported development and implementation of a NO<sub>x</sub> prediction model (operations monitoring program) in a 40 CFR 60, Subpart Db industrial boiler was in 1988.<sup>5</sup> The prediction system for an auxiliary boiler at a power plant is still in use today, without modification.

Parametric monitoring (PM) is the monitoring of the operation of an emission unit or piece of pollution control equipment in order to estimate the emission rate. One example of parametric monitoring can be found in Appendix E.<sup>6</sup> Appendix E is the optional NO<sub>x</sub> emission estimation protocol for gas-fired and oil-fired peaking units. The procedure begins with NO<sub>x</sub> emission testing at four load ranges using EPA Reference Test Methods.<sup>7</sup> A fuel specific curve of the test results is developed as shown in Figure 1. This figure represents a graph of NO<sub>x</sub> (lb/million Btu, HHV) versus fuel heat input (million Btu/hr,

HHV), covering the minimum, maximum, and two interim load conditions. Below the minimum heat input point, the emission rate is assumed to be equivalent to the minimum load level. In order to determine the NO<sub>x</sub> emission rate for the unit, the heat input to the unit is determined using fuel flow measurements and the fuel heating value. The NO<sub>x</sub> emission level is then estimated by interpolation (calculated) between the two nearest heat input levels. A NO<sub>x</sub> emission rate (lb/hr) is calculated by multiplying the heat input (million Btu/hr) by the estimated emission level (lb/million Btu).

There are also “alternative” monitoring systems which have been developed to work in conjunction with continuous emissions monitoring systems. For a combined-cycle electric generating facility in Virginia, an alternative monitoring system was developed<sup>8</sup> to resolve the conflict of duct burner emission rates with 40 CFR 60, Subpart Da, limitations (duct burner rated at 266 million Btu/hr) and the gas turbine emissions regulated by 40 CFR 60, Subpart GG. The alternative system met the criteria of being able to demonstrate compliance at the same or higher stringency as the method or procedure specified in the regulations, and that the compliance with applicable emission limitations have been sufficiently demonstrated by other means to justify a testing waiver.

Another example of an alternative monitoring system is the backup calculation of ammonia slip from a combined-cycle cogeneration facility in New Jersey equipped with selective catalytic reduction (SCR) for NO<sub>x</sub> control. Since direct ammonia slip measurements have proven to be unreliable, an alternative set of calculations were programmed into the CEM data acquisition and handling system. The first calculation determined the ammonia calculation (ppmvd) in the inlet to the catalyst bed, followed by a second calculation which used SCR inlet NO<sub>x</sub> and stack outlet NO<sub>x</sub> concentrations along with the catalyst bed inlet ammonia concentration to predict a worst case ammonia slip.<sup>9</sup>

## THE PROS AND CONS

When regulations allow for use of alternative emissions systems, the key to using either predictive, parametric, or alternative monitoring techniques in lieu of continuous emissions monitoring is to select a system appropriate for the specific application. Obviously, for a gas-fired peaking unit, the use of the Appendix E parametric model to estimate NO<sub>x</sub> emissions is less expensive and easier to implement than either a PEM or a CEM system. If the parametric model, however, does not appear to be valid, one needs to take a step back and evaluate the problem. While Figure 1 represents actual test results for a gas-fired unit, an identical unit at the same facility showed more erratic results as seen in Figure 2. Closer investigation revealed that the unit control system for the sister unit required adjustment at the 150 million Btu/hr heat input level.

Often times the use of a parametric monitoring system is preferable to a CEM system. An example of this involves a solvent recovery system associated with a stencil coating operation. The composition of the stencil coating is toluene, ethyl acetate, isopropyl alcohol, and ink grind. The air permit requires the use of control equipment with an overall volatile organic material (VOM) capture efficiency of greater than 81%. The total hydrocarbon monitoring system installed at the inlet and outlet of the carbon beds measures the recovery efficiency across the system, but does not provide a measurement of overall capture. To account for fugitive VOM emissions and overall capture efficiency, the site uses mass balance calculations using inlet flow rates to the stencil process, in conjunction with recovered solvent flow rates, resulting in an accurate determination of VOM emissions and capture efficiency. Furthermore, gas chromatographic analysis of the recovered solvent composition versus the stencil coating composition allows the source to calculate the emissions of toluene (a hazardous air pollutant),

ethyl acetate, and isopropyl alcohol. This additional set of calculations evaluates the effectiveness of the carbon beds recovering the various components.

### Other Issues

**Cost.** The first consideration in the development, installation, and operation and maintenance (O&M) of a PEM or PM system is cost.<sup>2</sup> Furthermore, the O&M on a PEM or PM system can be significantly reduced in comparison to a CEM system. The need for calibration gases, cylinder gas audits, CEM spare parts, emergency repair service, CEM training of instrument technicians, and “trips up the stack” will be eliminated.

On the other hand, poor timing or equipment selection can greatly affect the overall PEM or PM cost of a project. In one installation, a PEM model was built using emissions data from a temporary test trailer and boiler operating data. The prediction model had an R-square value (square of the correlation coefficient) better than 0.95, with a spread of residuals (predicted NO<sub>x</sub> - actual NO<sub>x</sub>, ppmvd at 3% O<sub>2</sub>) generally within  $\pm 2$  ppmvd across the load range. Approximately two weeks later, the model was programmed into the boiler data acquisition system and a relative accuracy test audit (RATA) was scheduled. Prior to conducting the actual audit, the facility noticed that the model was predicting NO<sub>x</sub> levels three to four times higher than expected. Closer examination of the problem revealed that the plant made a decision to replace all boiler instrumentation after completion of the test program. This was contrary to guidance contained in the PEM model building protocol which called for all controls to be calibrated prior to the start of the test program. Their decision was made with the best intentions--they felt that since the boiler would have a new system for predicting emission rates, the boiler controls should be upgraded to what was considered state-of-the-art. The first predictive emission model, therefore, was based on data obtained from erroneous boiler controls (i.e., unreliable and uncalibrated), rather than the new “calibrated” controls. A second NO<sub>x</sub> prediction model was developed with the new controls and the unit easily passed the RATA test (< 1.5% RA). The overall cost for the development of this particular PEM system probably approached the cost of a CEM system.<sup>10</sup>

The data acquisition and handling system (DAHS) is another area where significant cost savings can be realized. At the top end of the spectrum are vendors that provide a complete turnkey package that includes the DAHS unit with all software required for reporting, recordkeeping, input parameter validation, and model building. At the other end of the spectrum are the end-users that prefer to utilize their own existing DAHS software, using a prediction model developed by others. Most new boilers and gas turbine installations, for example, already have a powerful PC-based DAHS capable of retrieving all essential unit operating parameters and performing calculations. With some programming effort by an in-house person, the source can be totally in control of their own software and not have to rely on a software maintenance contract with a vendor. A third option is to have the model building performed by one vendor, with another vendor supplying the DAHS.

Further enhancements to an existing CEM DAHS can also be considered. For example, at one combined-cycle cogeneration facility in the midwest, the air permit requires a CEM system for NO<sub>x</sub> and CO from the gas turbine unit, but allows the use of predictive NO<sub>x</sub> emissions for the two 40 CFR 60, Subpart Db auxiliary boilers. In discussions with one CEM system integrator/software vendor,<sup>11</sup> all boiler operating parameters could be read from the facility’s distributed processing control system data highway and integrated into the CEM DAHS. The NO<sub>x</sub> models for the boilers can then be added as calculated data channels requiring only minor programming changes.

**Model Building.** Whether a model is developed using first-principles, regression models, or non-linear models, all systems employ some form of empirical analysis using data collected from actual emissions measurements and concurrent unit operating parameters. No model can be developed without adjustment based on empirical data. Therefore, since these models are more data-intensive rather than knowledge-intensive, the more “valid” data you have for analysis, covering the full range of operating conditions, the more powerful the model. A carefully planned test program will cover all operating loads and operating conditions. In most cases, adjustments in flue gas recirculation rates will affect boiler NO<sub>x</sub> emissions. Yet, for one Subpart Db industrial boiler in California, emissions measurements for the model development were taken at 2.5 to 5% load increments from the minimum load condition at 10% (10:1 turndown) up to 105% load (slightly overfiring the unit). Since the unit had fuel-induced flue gas recirculation (FGR), not forced FGR, FGR flow was not a statistically significant variable in the prediction model developed for the unit.

Computer programs used for the development of predictive emissions monitoring algorithms are extremely powerful, but can be misused. If a database contains measured emissions data and concurrent operating data for ten or twenty operating parameters, that doesn't mean that all twenty parameters should be used in the final model. Only statistically significant parameters that contribute to the predictive ability of the model should be used in the PEM system. In the evaluation of the California Subpart Db boiler mentioned above, one model was evaluated for the entire load range had an R-square > 0.975 with only one operating parameter, and showed a slight improvement (R-square > 0.9907) when two other parameters were added to the model. Figure 3 represents a scatter plot of the results for the three-variable model, and Figure 4 illustrates the distribution of residuals (predicted-actual NO<sub>x</sub>) across the entire load range. To further improve the model, the source has the option of developing a part load model covering loads below 5:1 turndown, or adding an additional statistically significant variable or two to further enhance the predictive power of the model at low load.

Start-up and shutdown emissions is evaluated as a separate data routine.<sup>10</sup> Given the transient nature of unit start-ups and shutdowns, a constant emission rate (e.g., lb/million Btu) is determined via stack testing and used as a constant when the unit is climbing to the minimum operating load (during a start-up), or dropping below minimum load (during a shutdown).

For dual-fuel units capable of performing on-line fuel transfers, another type of transient condition exists that needs to be evaluated. Since a predictive algorithm for a fuel transfer would not be very reliable, a separate emission rate constant for a fuel transfer is recommended.

**Alternative Monitoring Under 40 CFR 75, Subpart E.** 40 CFR 75, Subpart E<sup>6</sup> has specific guidelines that must be met for approval of an alternative emissions monitoring system to predict emission rates. Subpart E requires that the predictive emissions monitoring system have the same or better precision than a CEM system, and also requires that the model accuracy be verified over 720 hours (30 days) of testing. This requires that 30 days of stack emission results be collected and compared with the PEM system model results. While the 30 day demonstration period for comparing actual emission data versus model results can be achieved on a plant with an existing CEM system, it may be cost prohibitive to utilize an emissions testing vendor for the duration of time necessary for model building and model validation.<sup>1</sup> Before drawing any conclusion, a 40 CFR 75 source desiring to develop predictive emissions monitoring system needs to thoroughly investigate the cost of the PEM system development and verification. The ongoing benefits of a PEM system (less O&M than a CEM, less personnel training, higher availability) may outweigh the development cost.

**Malfunction Conditions.** No matter how much data has been collected to build a prediction model, which may have covered almost every imaginable operating scenario, there will still be malfunction conditions which will effect emission levels in a manner that cannot be predicted. For example, in a gas turbine which utilizes water injection for NO<sub>x</sub> control, CO emissions will typically vary from about 400 ppmvd at minimum load (30%) to <10 ppmvd at base load (100%). One of the parameters measured in a gas turbine with a can-annular arrangement of combustors is blade path spread (BPS). BPS is the difference between the average blade path temperature and the individual blade path temperature which is farthest from the average. In other words, if the average of 14 sets of blade path thermocouples was 800 °F, and the farthest reading from the average was 845 °F, then the BPS value would be 45 °F. Typical BPS levels range from 15 to 50 °F during normal operation, with a trip point set at approximately 90 °F. Should one or more of the water injection nozzles become plugged, or water distribution throughout the combustor baskets becomes uneven, then the BPS value will climb. As a direct consequence, CO emissions can increase significantly, and unpredictably. A BPS value of 65 °F at 70% load on one day may translate into 300 ppmvd CO, and a day later the same 65 °F BPS value at 70% load, with similar ambient meteorological conditions, could result in actual CO levels of over 500 ppmvd.

There are ways around the dilemma. By using routines such as input parameter validation, boundaries are set for certain operating parameters that can have an effect on emission rates. If the unit operates outside of the boundaries determined during the model building effort, then an alarm could flag the data as questionable.

In the BPS case mentioned above, problems could also have occurred if the unit was equipped with a CEM system. If the unit had a CO monitor with a range from 0-500 ppmvd, and the BPS value climbed above the normal operating range, it is possible that CO emissions would exceed the 500 ppmvd level and not be monitored by the CEM system.

Malfunction conditions and off-normal operating conditions will occur on occasion, and they will contribute to excess emissions. When these situations occur, they may be unmeasurable (for the CEM analyzer range) and unpredictable (outside the boundaries established during the model building). Prompt investigation and corrective action in accordance with air permit conditions is necessary regardless of the type of monitoring system employed at the facility.

**PEM as a CEM Backup.** For facilities with existing CEM systems, one may wish to consider development of a PEM system for use as a backup to the CEM system. In the event of monitor failure, or excessive drift, a predicted emission rate is preferable to no data at all.

**Sulfur Dioxide.** Many facilities calculate SO<sub>2</sub> emission rates from fuel flow, fuel heating value, and fuel sulfur contents. Since the molecular weight of sulfur is 32, and the molecular weight of sulfur dioxide is 64, every pound of sulfur contained in the fuel is theoretically converted to two pounds of SO<sub>2</sub>. Therefore, to determine daily and annual SO<sub>2</sub> emissions using fuel sampling and analysis, representative fuel samples can be collected and analyzed daily.

Direct emission measurements of SO<sub>2</sub> at coal-fired units with SO<sub>2</sub> analyzers, in conjunction with exhaust flow rate monitors, will often result in SO<sub>2</sub> emissions (lb/hr) that are higher than the theoretical values calculated from fuel sampling and analysis. This discrepancy is typically related to inaccuracies in continuous exhaust flow measurement techniques, rather than the SO<sub>2</sub> analyzers.<sup>12</sup> For example, if the fuel sulfur content of the coal supply is 0.65% by weight, with a heating value of 9,650 Btu/lb (HHV), a

heat input of 3300 million Btu/hr would result in a maximum emission rate of 4,446 lb/hr (using 100% conversion of sulfur to SO<sub>2</sub>). If the actual sulfur conversion was 97%, then the corresponding emission rate would be 4,313 lb/hr. If the CEM system and exhaust flow rate monitor were operating without error, the measured SO<sub>2</sub> emission rate should agree with the 4,313 lb/hr rate determined from the fuel analysis. But if the exhaust flow monitor reads 7% high, the CEM system would erroneously calculate an SO<sub>2</sub> emission rate of 4,614 lb/hr.

When SO<sub>2</sub> emissions monitoring is required, especially for units affected by the Acid Rain Program, it is advisable to continue evaluation of the CEM readings in comparison to the fuel sampling and analysis alternative.<sup>12</sup>

**Carbon Monoxide Prediction.** There is much debate concerning whether or not a predictive emissions model could be developed for carbon monoxide emissions. In one set of studies,<sup>13</sup> CO emissions were successfully predicted for a gas turbine and an ethylene furnace using the non-linear regression methods. In two other studies,<sup>1</sup> non-linear techniques were used for two gas turbines and both units failed to pass the correlation test. The reason for failure was primarily the low CO emission levels observed in the latter study. With a CO analyzer set at a range from 0 to 100 ppmvd, and a gas turbine emitting levels in the 0-1 ppmvd range during normal operation, the inherent inaccuracy of a CO analyzer is greater than the level being measured, and makes it virtually impossible to pass the correlation test on a regular basis. This issue has been considered by some regulators, where all statistical tests may be waived, including the correlation test, if the average emission levels are below 10 ppmvd.

**Particulate Emissions.** In exactly the same manner as in 40 CFR 75, Appendix E, for generating NO<sub>x</sub> prediction curves, particulate emissions can be determined and plotted. As shown in Figure 5 for a hypothetical oil-fired boiler without particulate emission controls, particulate emission rates (lb/million Btu) measured at various load points could be used to calculate particulate emissions (lb/hr) with simple multiplication. This approach requires accurate fuel flow metering, as well as an evaluation of the unit operating parameters that may affect particulate emissions. In this example, even though the emission rate (lb/million Btu) was slightly higher at part load, the particulate emission level (lb/hr) associated with part load operation was significantly less than the level corresponding to full load.

For coal-fired units with electrostatic precipitators (ESP) for particulate control, computer programs have been developed<sup>12</sup> to determine allowable load (MW) versus emissions (lb/million Btu) in the event that there is a malfunction of the control equipment. For example, on a unit with an ESP configuration 4 cells deep by 8 sections wide, the program's calculation may show that the loss of one section will still allow the unit to operate at full load and remain in compliance with the particulate limit, but the loss of two sections would require a unit derating until the malfunction condition was repaired.

## MAINTENANCE

Predictive and parametric monitoring systems rely on operating parameters to calculate emission rates. If the computer model utilizes invalid or erroneous input parameters, the resulting emissions prediction will also be in error. Therefore, any facility using PEM and PM systems should have a quality assurance and quality control program in place to periodically check and calibrate the applicable instrumentation.

## CONCLUSION

Predictive, parametric, and alternative emissions monitoring systems all have a valid place in regulatory compliance. The key to success for any installation is the selection of the most appropriate method for a particular application. In many cases, alternatives to CEM systems are more accurate and provide more valuable information. Engineers have developed many creative solutions for demonstrating regulatory compliance on a continuous basis.

There is no single modeling technique which is preferable for predictive emissions monitoring systems. Models based on first principles, regression techniques, and non-linear methods all have the potential to pass relative accuracy test criteria. Successful use of predictive techniques requires high-quality input parameters for use in the calculations. All metering, whether it is for fuel flow, flue gas damper positions, air flow, temperature readings, in situ oxygen sensors, steam flow measurements, pressure gauges, and other instrumentation can drift over time. A well conceived quality assurance program with periodic calibration checks on the metered parameters will help ensure the development of, and continued operation of, a reliable predictive emissions monitoring system.

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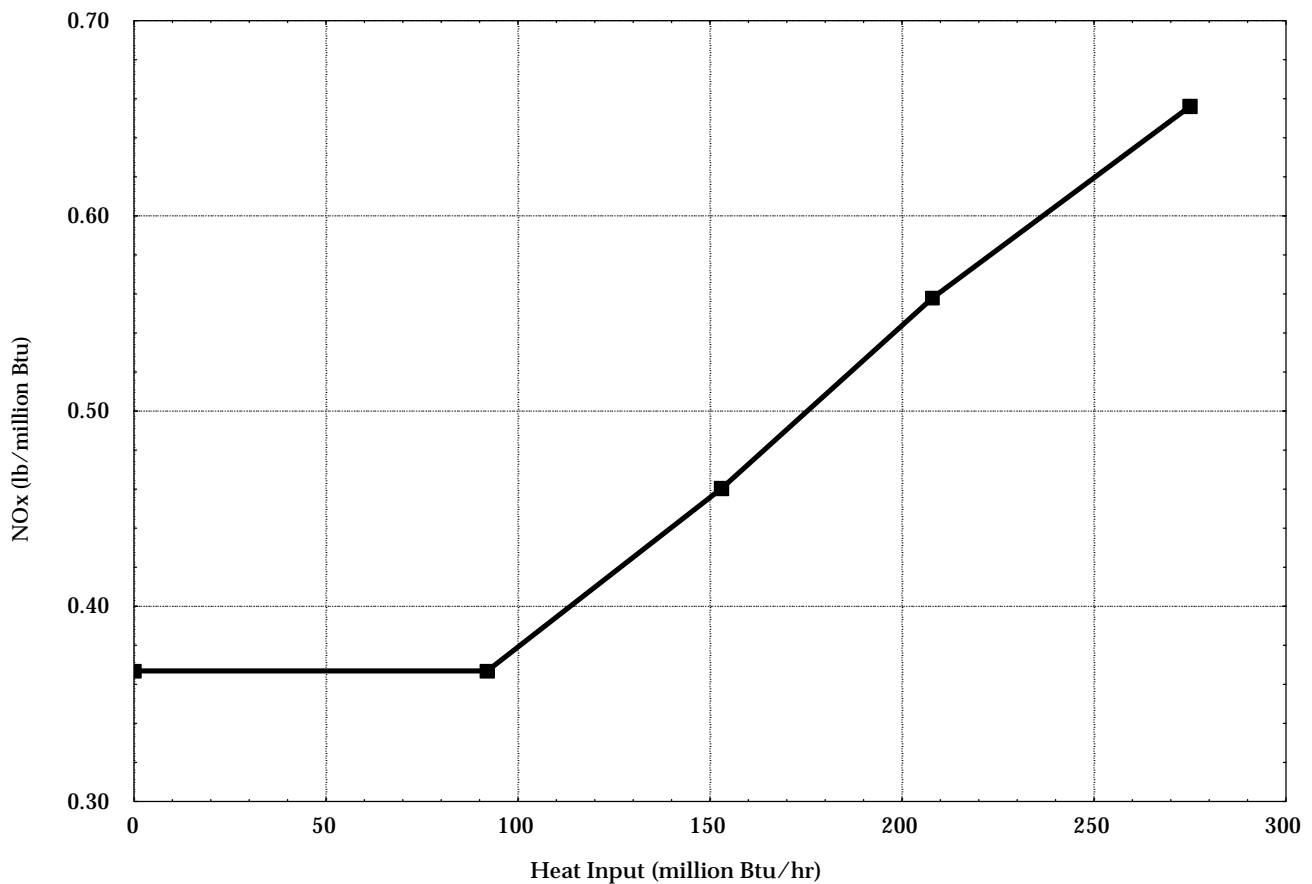


Figure 1. Graph of NO<sub>x</sub> (lb/million Btu) versus Heat Input (million Btu/hr) for a Peaking Unit Firing Natural Gas to Comply with Appendix E of 40 CFR 75; Valid Data.

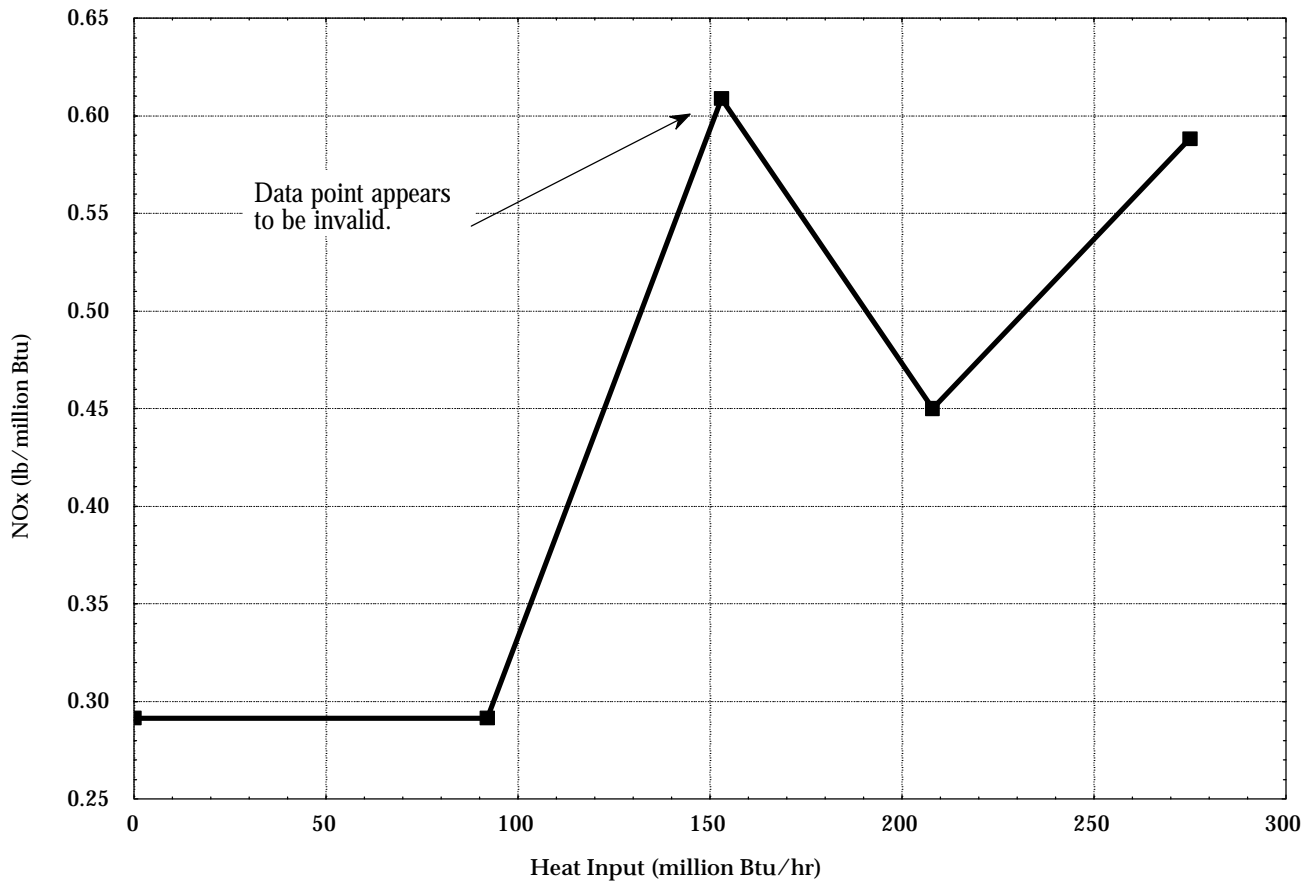


Figure 2. Graph of NO<sub>x</sub> (lb/million Btu) versus Heat Input (million Btu/hr) for a Peaking Unit Firing Natural Gas to Comply with Appendix E of 40 CFR 75; Questionable Data.

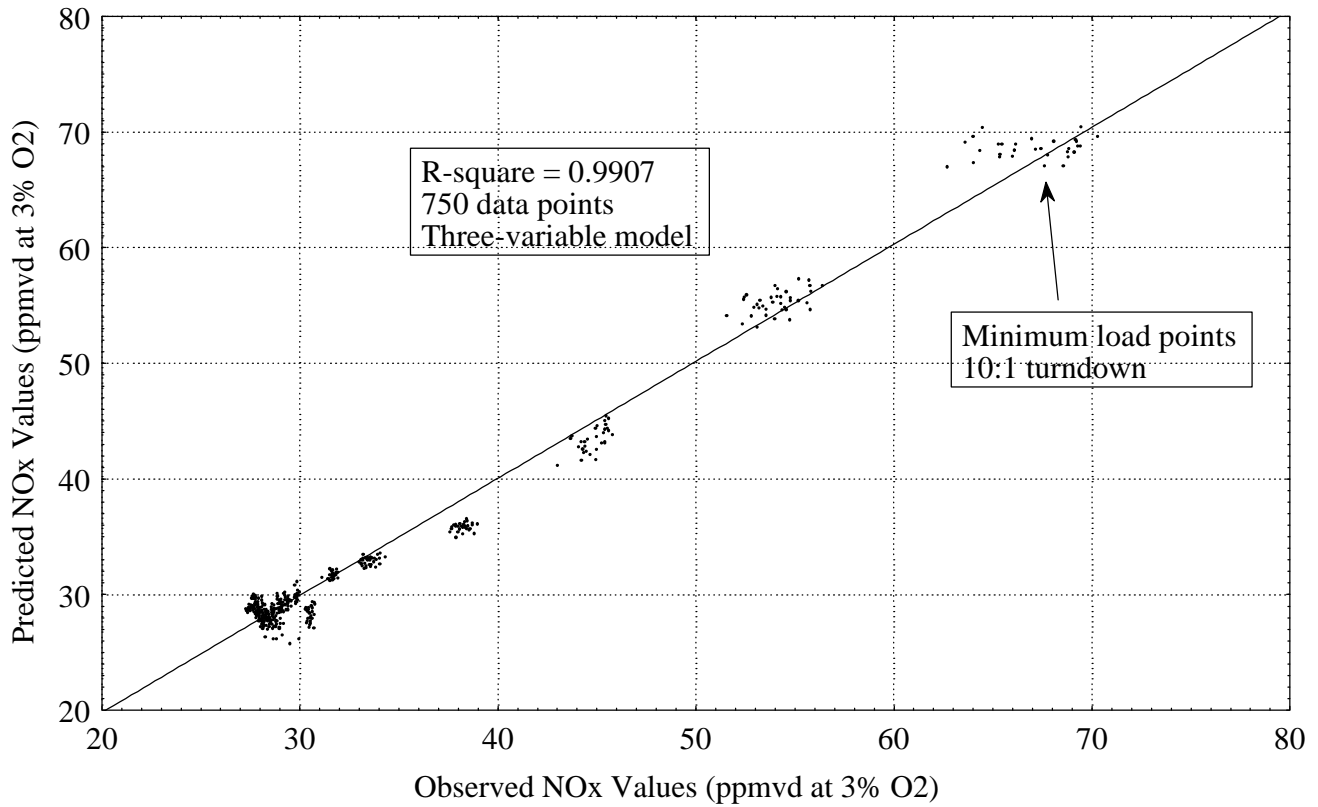


Figure 3. Scatter Plot of Predicted versus Actual NO<sub>x</sub> (ppmvd at 3% O<sub>2</sub>) for a Three-Variable NO<sub>x</sub> Prediction Model Covering the Full Load Range of a Subpart D<sub>b</sub> Industrial Boiler Firing Natural Gas.

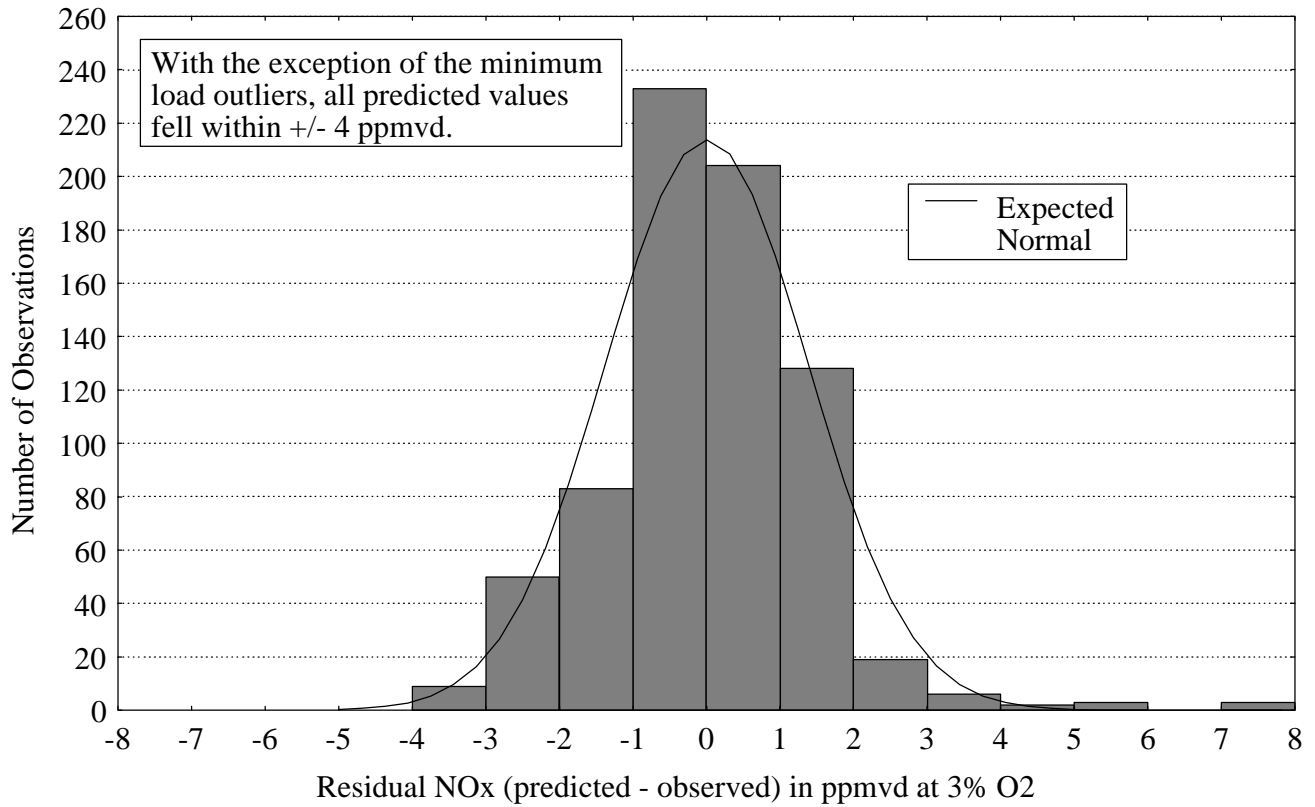


Figure 4. Plot of Residuals (Predicted-Actual NO<sub>x</sub>) for a Three Variable NO<sub>x</sub> Prediction Model Covering the Full Load Range for a Natural Gas-Fired Subpart Db Industrial Boiler.

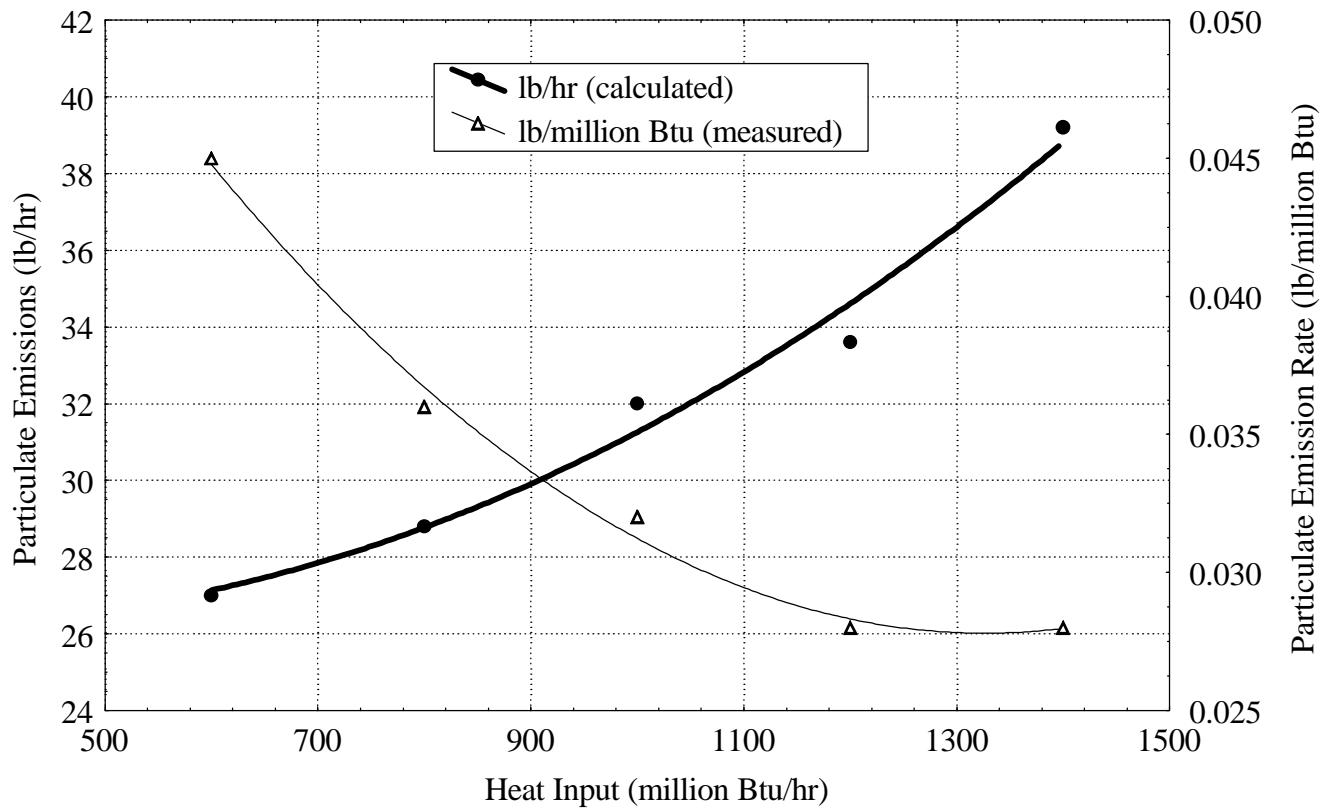


Figure 5. Plot of Particulate Emissions (lb/hr [left axis]; lb/million Btu [right axis]) versus Heat Input (million Btu/hr) for an Oil-Fired Peaking For Use in a Parametric Monitoring System to Continuously Calculate Particulate Emission Rates.