Developing Real-Time Emissions Estimates for Enhanced Air Quality Forecasting

Jeongran Yun[1], Prakash Doraiswamy[2], Christian Hogrefe[3], Eric Zalewsky[4], Winston Hao[4], Jia-Yeong Ku[4], Mark Beauharnois[1], and Kenneth L. Demerjian[1]

1 Atmospheric Sciences Research Center, University at Albany, Albany, NY

2 RTI International in Research Triangle Park, NC

3 Atmospheric Modeling and Analysis Division, National Exposure Research Laboratory, U.S. EPA in Research Triangle Park, NC

4 New York State Department of Environmental Conservation in Albany, NY

Corresponding author: Kenneth L. Demerjian, kdemerjian@albany.edu

Background and Objective

The operation of air quality forecast models (AQFMs) based on coupling a numerical weather prediction (NWP) model to an emissions processor and a chemical transport model (CTM) are now common within the U.S.[1-8] Health professionals and air quality managers utilize these forecasts to alert susceptible populations and the public at large of poor air quality conditions and recommended actions to minimize exposures. In addition, air quality forecasts have the potential of guiding emission interventions designed to mitigate episodic events and exceedances of National Ambient Air Quality Standards (NAAQS).

While the NWP component of such AQFMs incorporates a large amount of real-time information in the form of initial conditions and analysis fields, the emissions processor often relies on simplifying assumptions about the magnitude and temporal - spatial variation of emissions. NOx and SO_2 emissions from major point sources are directly measured, tracked and archived via the U.S. Environmental Protection Agency (EPA)'s continuous emissions monitoring (CEM) network in support of the Clean Air Markets Division for emission cap and trade programs. Unfortunately it is not feasible to incorporate these emission measurements in real-time into AQFMs.

The development of an approach to enhance short-term emission estimates is expected to improve the overall performance of AQFMs and specifically the performance associated with episodic events. The inherent relationships between weather fluctuations, electricity demand, emissions, and air quality are not currently represented in the emissions processing module of AQFMs. We explore the relationship between ambient temperature, energy demand and electric generating unit (EGU) point source emissions and potential techniques for incorporating real-time information on the modulating effects of these variables on EGU emissions using the Mid-Atlantic/Northeast Visibility Union (MANE-VU) region as an example.

Enhanced Emissions Estimates

The emissions model applied in AQFMs typically derives emissions from annual totals of emitted species by source category that are allocated monthly and then hourly based on averaged temporal profiles. Some source categories, such as EGUs exhibit significant daily variations in emissions as compared to their means, especially during periods of peak electrical power demand. Point source emissions are measured and archived as part of the U.S. EPA network of CEMs and in support of the Clean Air Markets Division emissions cap and trade program (http://www.epa.gov/captrade/). The archived hourly averaged data are typically available within a year of collection and are also used to refine emissions inventories for NAAQS modeling in State Implementation Plans (SIP). The variation in EGU emissions can be observed by comparing their “actual” and “average” hourly emissions, where “actual” refers to measured hourly emissions from CEMs for EGUs on a unit by unit basis and “average” refers to the hourly emissions derived from annual emission totals using averaged temporal profiles (i.e., monthly, daily, and hourly profile) based on the actual 2007 CEM data on a state-by-state basis within the MANE-VU region.[9]

Figure 1 shows the time series of daily emissions for the “actual” and “average” nitrogen oxides (NO_x) emissions in tons/day during summer of 2007. The average emissions show the monthly and weekday – weekend patterns used in their allocation of the annual emissions; Figure 2 shows the extent to which the “actual” and “average” NOx emissions differ on a daily basis. Differences in EGU emissions typically occur on days of high energy demand which is associated with high ambient temperatures.

On days of high energy demand, additional generators are brought online for power generation. These units are usually referred to as "Peaking Units" and typically operate less than 15% of the time during a year.[10] Figure 3 shows the NOx emissions from "Peaking Units" in the MANE-VU region from May to September 2007. It illustrates the significant contribution from peaking unit emissions can have on some days. It should be noted that, depending on federal and state reporting requirements, not all "Peaking Units" may be equipped with CEM and, therefore, cannot be considered in this analysis.

Preliminary air quality modeling studies indicate that time periods when the "actual" emissions were larger than the "average" emissions (i.e., positive difference) usually coincided with days leading to high ozone (O_3) concentrations.[11] The impact of differences in point source NOx emissions between the two scenarios on O_3 predictions varied by location, with the largest changes at the grid cells adjacent to the affected point sources. The maximum difference in 1-hr or 8-hr daily max O_3 was typically greater than 4 ppb around the Ohio River valley, and less than 2.5 ppb in general. Differences as large as 8 to 10 ppb were noted at selected monitor locations in the MANE-VU region, illustrating the need for refined emissions in air quality modeling. In the following section, we present an example approach of incorporating the relationships between energy demand and emissions into AQFMs.

Energy Demand Forecasts and Enhanced EGU Emissions Estimates

Regional Independent System Operators (ISOs) perform daily energy forecasts as part of their mission to ensure efficient generation and flow of power to satisfy energy demand and administer electricity markets. These forecasts are typically available online on their website. ISOs in operation within the eastern US include: the New York ISO[12], the New England ISO[13], the Midwest ISO[14], the PJM Interconnection[15] and the Southeastern Electric Reliability Council[16]. The availability of real-time energy load forecasts in principle provides an opportunity to enhance real-time EGU emissions estimates for AQFMs.

For example, a comparison of 2007 CEM NOx emissions and NYISO forecast energy load data shown in Figure 4 indicates a robust correlation between these variables. In addition, a comparison of actual and forecast energy load data from this same period (not shown) reports a correlation coefficient of $R^2 = 0.954$, indicating that load forecasts provide an opportunity to improve daily EGU emission estimates.

Incorporating emissions from peaking units on a real-time basis requires taking into account the relationship of between meteorology, energy demand and EGU unit operation. The dominant meteorological parameter affecting the energy demand forecast is temperature.

Energy Load Adjusted EGU Emissions Estimates

Historical power load data from the NYISO archive[12] and temperature observations data from the research data archive[17] at the National Center for Atmospheric Research have been analyzed for statistical relationships between daily power load and average temperature in NY State.

Figure 5 shows a quadratic relationship between ozone season temperature data (May-September) from 2007 to 2009 and the actual power load for the NYISO region aggregated over NY State. The regression model is: power load (MW) = $288.6112x^2 - 2.9463E{+}4x + 1.1487E{+}6$ Where, x = average daily temperature (which ranged from 45 to 81^{o}F) and $R^2 = 0.7554$.

A comparison between the model predicted power load using the above relationship and the actual power load for 2010 is shown in Figure 6 with an R^2 of 0.8039. A similar comparison for 2011 (not shown) had an R^2 of 0.8113. Since the results indicate reasonable performance of the regression model, the correlations can be employed to support a better forecast. As the range of daily average temperatures during 2007 to 2009 for the model development was up to 81 °F, predictions of power load at temperatures above 81 °F suggest possible over prediction and the potentially greater influence of EGU peaking units.

Although energy load is distributed across ISO regions and across states, energy use within a region does not necessary reflect where the power is generated and thus where emissions occur. If a significant portion of the electric generation to meet load demand occurs outside of the aggregated ISO domains, the relationship between forecasted load and EGU emissions will be more uncertain. In addition, EGU emissions will vary over the years due to emission controls and changes in electric generation capacity and load demand; the latter very likely affecting the operating frequency of peaking units.

Methodologies for Incorporating Real-Rime EGU Emissions Estimates in AQFMs

Current analyses indicate that two methodologies look feasible for incorporating real-time EGU emissions estimates in AQFMs. The first approach considers aggregating (by state) the hourly energy load forecast data (day 2) from the ISOs for pre-processing by the Sparse Matrix Operator Kernel Emissions (SMOKE) processor.[18] The SMOKE preprocessing will involve incremental adjustments of EGU unit emissions at the state level and on daily average basis, reflecting the statistical relationship between previous years' energy load and emissions data.

The second approach draws from the relationship between temperature – energy load and EGU emissions and is more indirect, but also does not rely on the ISOs real-time energy load forecasts. In this case forecasted temperatures used to process other emission components in the SMOKE emissions model will be applied to the statistical relationship between previous years' daily average temperatures and actual energy load data by state. As temperature has been shown to be a reasonable surrogate for energy load, using a direct relationship between temperature and EGU emissions is also feasible. In either case, similar procedures for the SMOKE preprocessing of the ISO energy load in relation to emissions would be followed.

Future Challenges and Outlook

AQFMs are being used by air quality managers and health officials to issue air quality advisories. Improving the accuracy of air quality forecasts will translate into providing more precise warnings to the public. In this article, we presented an example of possible approaches to refine the characterization of emissions from power plants in AQFMs. We explored relationships between ambient temperature, energy demand and EGU point source emissions and suggested methodologies for applying these relationships to enhance real-time EGU emissions estimates for use in AQFMs. However, there are some limitations.

- While the relationships presented here are robust, they were developed based on aggregated emissions sources in NYS, and as such may be best suited to improve regional-scale predictions.

- Developing unit-specific relationships will be much more challenging because load forecasts are not available at that level, and economic and operational constraints likely are at least as important as meteorology in determining which unit runs on which day at which level.
- Finally, depending on federal and state reporting rules, some of the “Peaking Units” with relatively small annual emissions may not be required to have CEM. Therefore, their annual total emissions are currently included in the miscellaneous point source category inventory and no further information on their temporal variation is readily available. Getting a better representation of their temporal variability may be important for finer scale applications, but is a challenge that may need to be addressed in the future.

The potential of an air quality forecast system is its possible utility as a dynamic air quality management tool that can provide information on likely emission intervention strategies that can avoid air quality exceedances. Improving the accuracy of the model predictions through refinements such as that discussed in this article is an important step towards achieving that goal.

Disclaimer

Although this work has been reviewed and approved for publication by the U.S. Environmental Protection Agency, it does not reflect the views and policies of the agency.

References

1. McHenry, J. N.; Seaman, N.; Coats, C.; Stauffer, D.; Lario-Gibbs, A.; Vukovich, J.; Hayes, E.; Wheeler, N. The NCSC-PSU numerical air quality prediction project: Initial evaluation, status and prospects. Proceedings of the 11th Joint Conference on the Applications of Air Pollution Meteorology with the Air and Waste Management Association, Long Beach, CA, January 9-14, 2000; American Meteorological Society: 2000; 403-408.
2. McHenry, J. N.; Ryan, W. F.; Seaman, N. L.; Coats, C. J.; Pudykiewicz, J.; Arunachalam, S.; Vukovich, J. M. A real-time Eulerian photochemical model forecast system - Overview and initial ozone forecast performance in the Northeast US corridor. *Bulletin of the American Meteorological Society*, **2004,** *85*, 525-548.

3. Kang, D.; Eder, B. K.; Stein, A. F.; Grell, G. A.; Peckham, S. E.; McHenry, J. The New England Air Quality Forecasting Pilot Program: Development of an evaluation protocol and performance benchmark. *J. Air Waste Manag. Assoc.*, **2005,** *55*, 1782-1796.
4. Otte, T. L.; Pouliot, G.; Pleim, J. E.; Young, J. O.; Schere, K. L.; Wong, D. C.; Lee, P. C. S.; Tsidulko, M.; McQueen, J. T.; Davidson, P.; Mathur, R.; Chuang, H. Y.; DiMego, G.; Seaman, N. L. Linking the Eta Model with the Community Multiscale Air Quality (CMAQ) Modeling System to Build a National Air Quality Forecasting System. *Weather and Forecasting*, **2005,** *20*, 367-384.
5. McKeen, S.; Chung, S. H.; Wilczak, J.; Grell, G.; Djalalova, I.; Peckham, S.; Gong, W.; Bouchet, V.; Moffet, R.; Tang, Y.; Carmichael, G. R.; Mathur, R.; Yu, S. Evaluation of several $PM_{2.5}$ forecast models using data collected during the ICARTT/NEAQS 2004 field study. *J. Geophys. Res.*, **2007,** *112.*
6. Hogrefe, C.; Hao, W.; Civerolo, K.; Ku, J.-Y.; Sistla, G.; Gaza, R. S.; Sedefian, L.; Schere, K.; Gilliland, A.; Mathur, R. Daily Simulation of Ozone and Fine Particulates over New York State: Findings and Challenges. *Journal of Applied Meteorology*, **2007,** *46*, 961-979.
7. Doraiswamy, P.; Hogrefe, C.; Hao, W.; Civerolo, K.; Ku, J.-Y.; Sistla, G. A Retrospective Comparison of Model-Based Forecasted $PM_{2.5}$ Concentrations with Measurements. *J. Air Waste Manag. Assoc.*, **2010,** 1293–1308, doi:10.3155/1047-3289.60.11.1293.
8. Eder, B.; Kang, D.; Rao, S. T.; Mathur, R.; Yu, S.; Otte, T.; Schere, K.; Wayland, R.; Jackson, S.; Davidson, P.; McQueen, J.; Bridgers, G. A Demonstration of the Use of National Air Quality Forecast Guidance for Developing Local Air Quality Index Forecasts. *Bulletin of the American Meteorological Society*, **2010,** 313-326.
9. Mid-Atlantic Regional Air Management Associations. 2007 regional emissions inventory. http://www.marama.org/technical-center/emissions-inventory/2007-emissions-and-projections/version-3-2007-emissions-inventory.
10. Mid-Atlantic Regional Air Management Associations. *Analysis of 2007 Emissions from Power Plants and Other Large Combustion Sources in the Mid-Atlantic and Northeastern United States*; Technical Report for Mid-Atlantic/Northeast Visibility Union: March 2011. http://www.marama.org/RegionalEmissionsInventory/2007hourlypoint/FinalDoc_mar2011_Analysis_of_Hrly_CAMD_Emissions_Data.pdf .

11. Doraiswamy, P.; Hogrefe, C.; Zalewsky, E.; Hao, W.; Demerjian, K.; Ku, J.-Y.; Sistla, G. Impact of Temporal Fluctuations in Power Plant Emissions on Air Quality Forecasts. Presented at the 9th Annual CMAS Conference, Chapel Hill, NC, October 11-13, 2010.
12. New York Independent System Operators (NYISO) Home Page. http://www.nyiso.com/.
13. New England Independent System Operators (ISONE) Home Page. http://www.iso-ne.com.
14. The Midwest Independent System Operators (MISO) Home Page. https://www.midwestiso.org.
15. PJM Interconnection regional transmission organization (RTO) Home Page. http://www.pjm.com.
16. Southeastern Reliability Corporation (SERC) Home Page. http://www.serc1.org/Application/HomePageView.aspx.
17. Meteorological Development Laboratory, Office of Science and Technology, National Weather Service, NOAA, U.S. Department of Commerce. 1987, updated half-yearly. *TDL U.S. and Canada Surface Hourly Observations, daily 1976Dec-cont.* Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory. http://rda.ucar.edu/datasets/ds472.0.
18. SMOKE v2.7 User's Manual. http://www.cmascenter.org/smoke/.

List of Figures

Figure 1. Actual daily and average EGU NOx emissions in the MANE-VU region.

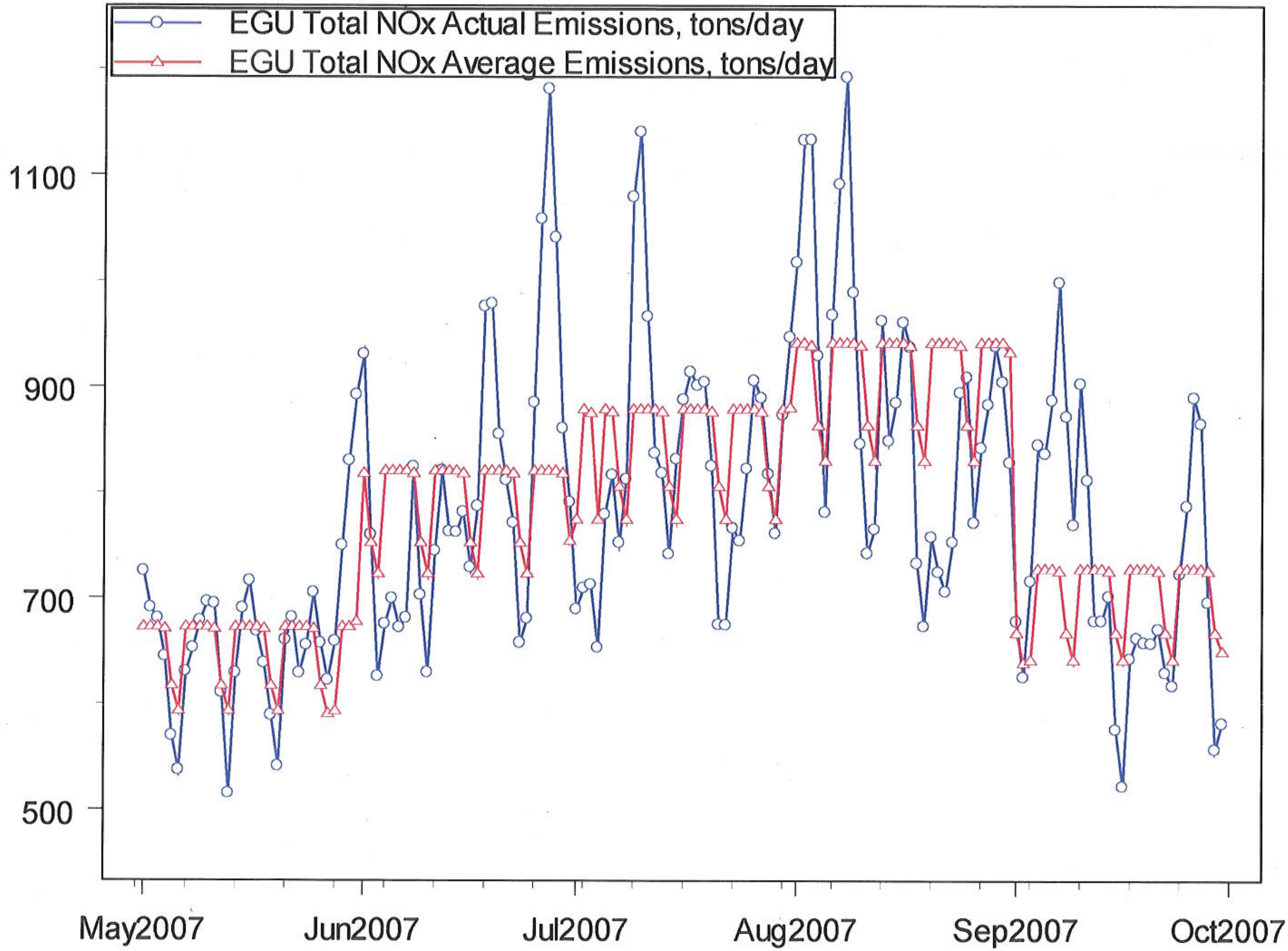
Figure 2. Difference in actual daily and average EGU NOx emissions in the MANE-VU region.

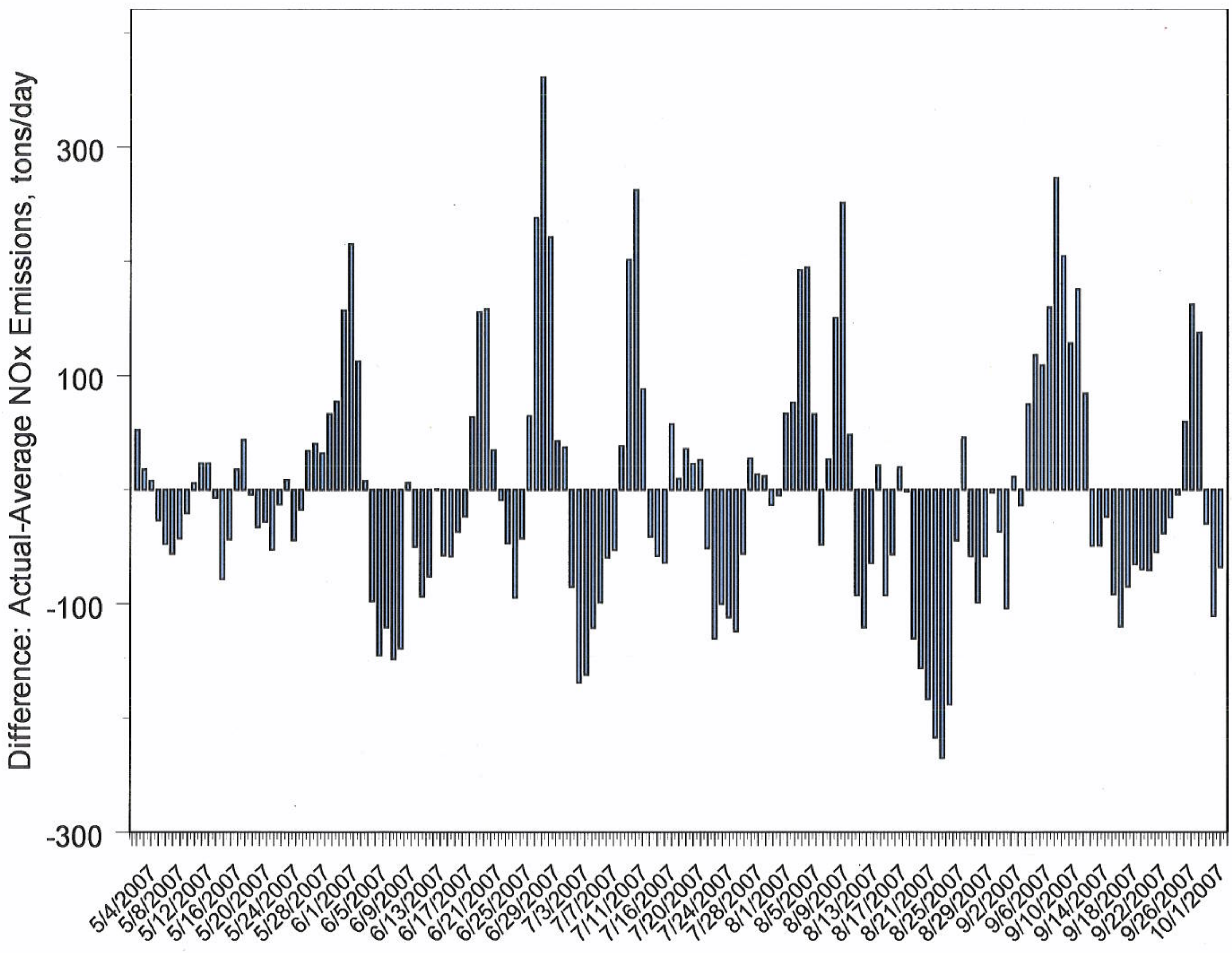
Figure 3. NOx emissions from "Peaking Units" in the MANE-VU region from May to September 2007.

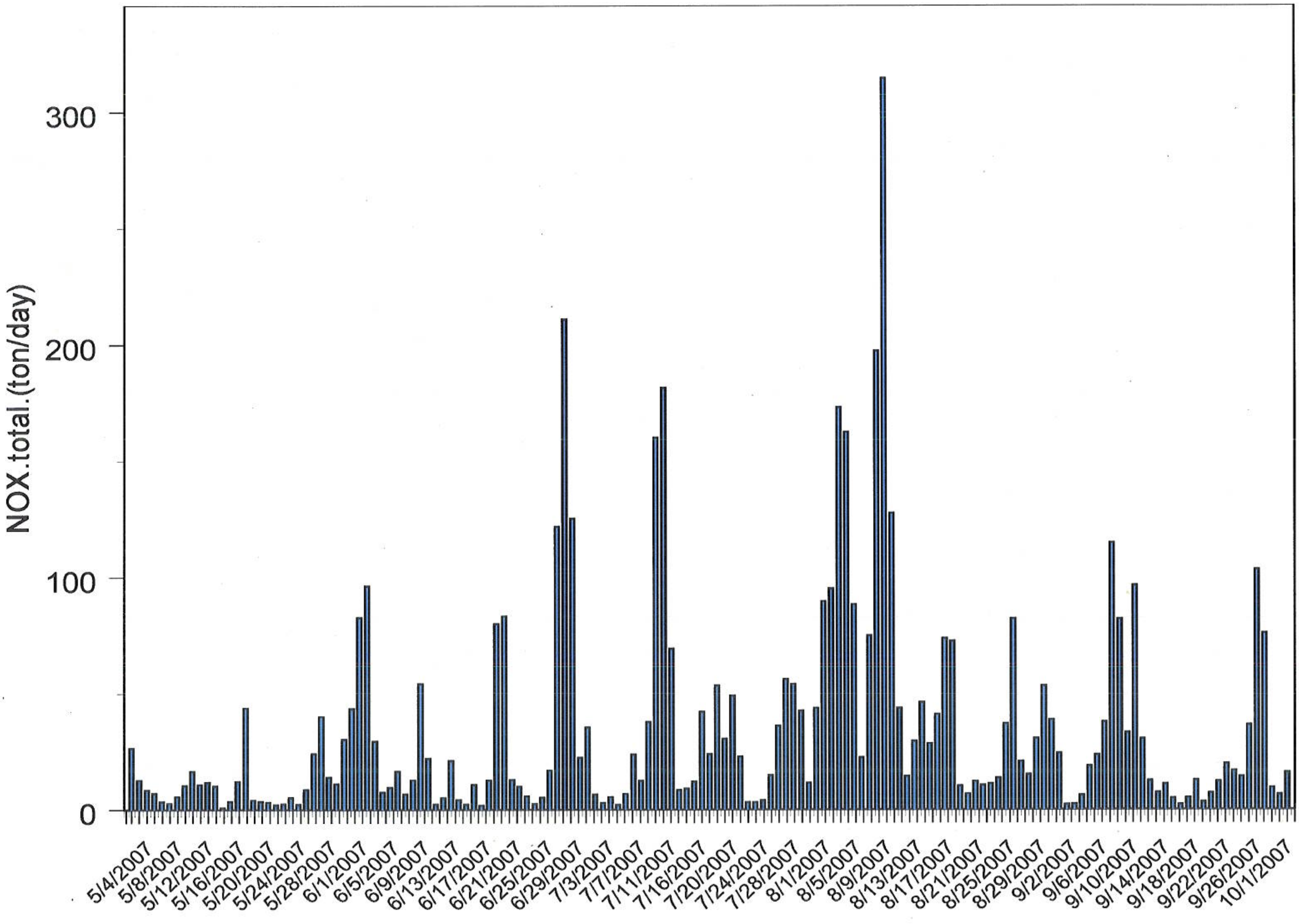
Figure 4. NYISO forecasted energy demand and actual daily CEM EGU NOx emissions in the MANE-VU region.

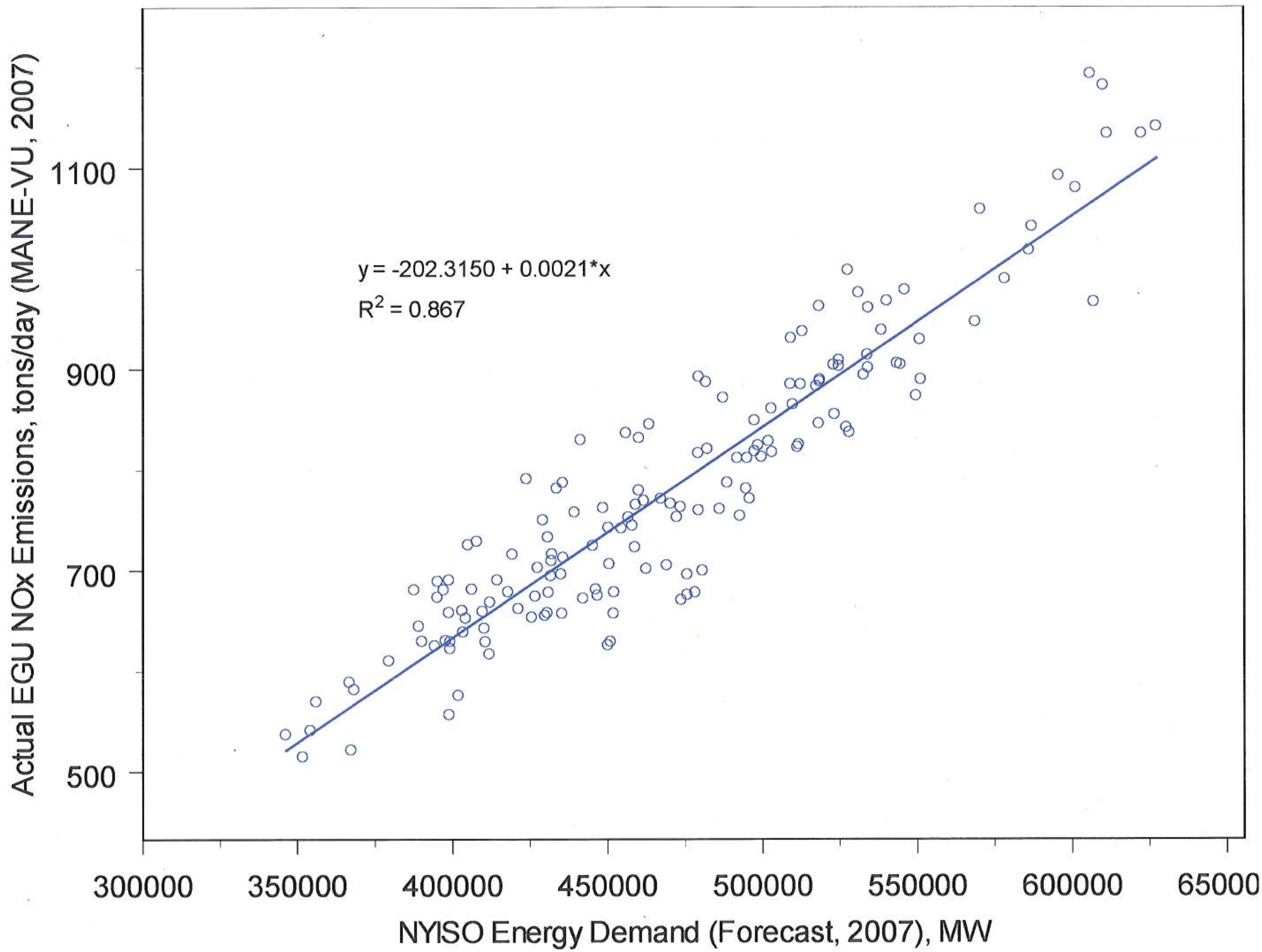
Figure 5. Regression model between NYISO actual power load (MW) and NY state wide daily average temperature (^{o}F) developed using ozone season data (May-September) from 2007 to 2009.

Figure 6. Prediction of 2010 power load with the regression model versus 2010 NYISO actual power load (MW)

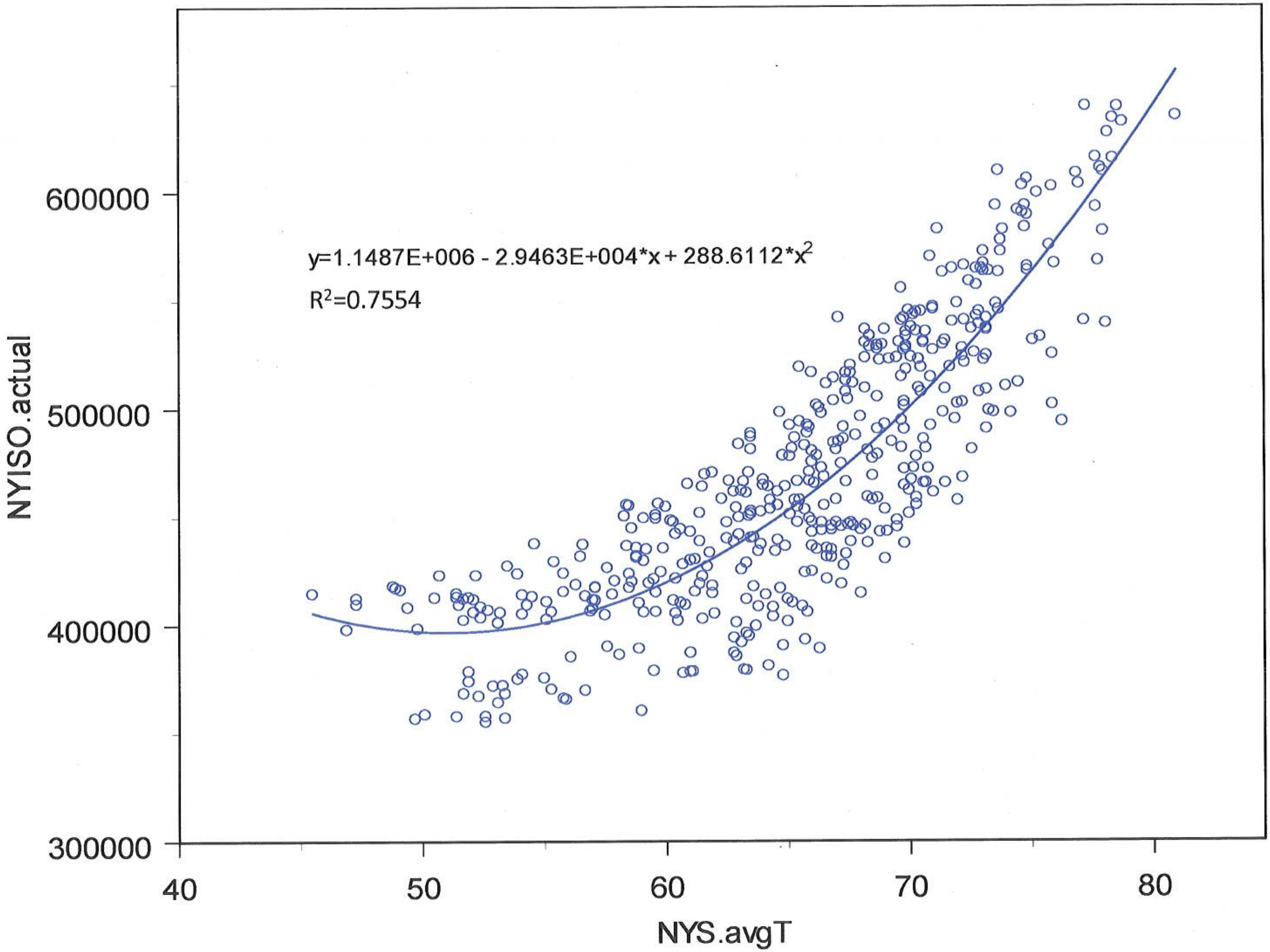

EGU Total NOx Actual Emissions, tons/day
EGU Total NOx Average Emissions, tons/day
1100
900
700
500
May2007
Jun2007
Jul2007
Aug2007
Sep2007
Oct2007

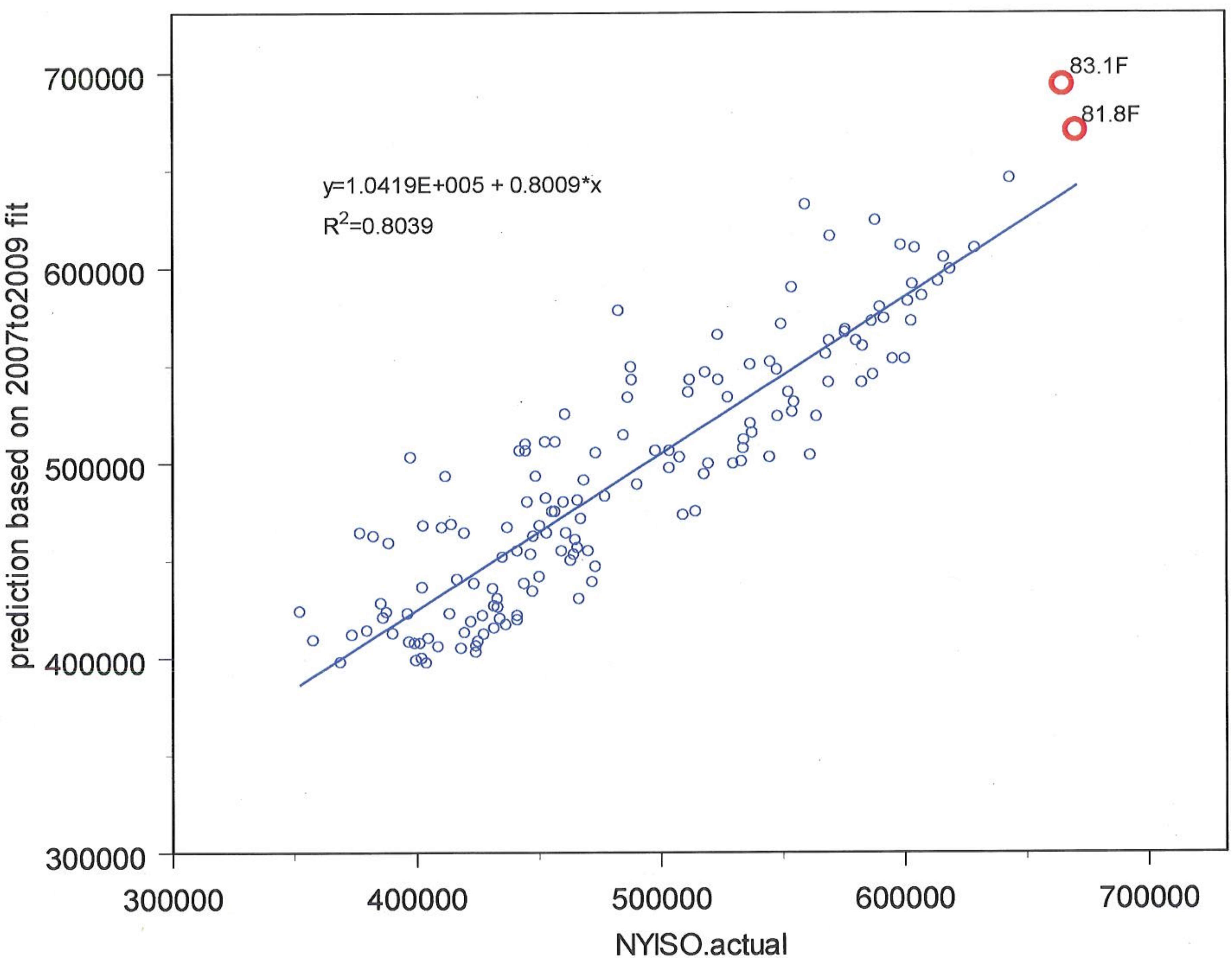

Difference: Actual-Average NOx Emissions, tons/day
300
100
-100
-300
5/4/2007
5/8/2007
5/12/2007
5/16/2007
5/20/2007
5/24/2007
5/28/2007
6/1/2007
6/5/2007
6/9/2007
6/13/2007
6/17/2007
6/21/2007
6/25/2007
6/29/2007
7/3/2007
7/7/2007
7/11/2007
7/16/2007
7/20/2007
7/24/2007
7/28/2007
8/1/2007
8/5/2007
8/9/2007
8/13/2007
8/17/2007
8/21/2007
8/25/2007
8/29/2007
9/2/2007
9/6/2007
9/10/2007
9/14/2007
9/18/2007
9/22/2007
9/26/2007
10/1/2007


NOX.total.(ton/day)
300
200
100
0
5/4/2007
5/8/2007
5/12/2007
5/16/2007
5/20/2007
5/24/2007
5/28/2007
6/1/2007
6/5/2007
6/9/2007
6/13/2007
6/17/2007
6/21/2007
6/25/2007
6/29/2007
7/3/2007
7/7/2007
7/11/2007
7/16/2007
7/20/2007
7/24/2007
7/28/2007
8/1/2007
8/5/2007
8/9/2007
8/13/2007
8/17/2007
8/21/2007
8/25/2007
8/29/2007
9/2/2007
9/6/2007
9/10/2007
9/14/2007
9/18/2007
9/22/2007
9/26/2007
10/1/2007



y = -202.3150 + 0.0021*x
R2 = 0.867
Actual EGU NOx Emissions, tons/day (MANE-VU, 2007)
1100
900
700
500
300000
350000
400000
450000
500000
550000
600000
65000
NYISO Energy Demand (Forecast, 2007), MW


y=1.1487E+006 - 2.9463E+004*x + 288.6112*x2
R2=0.7554
600000
500000
400000
300000
NYISO.actual
40
50
60
70
80
NYS.avgT


83.1F
81.8F
y=1.0419E+005 + 0.8009*x
R2=0.8039
700000
600000
500000
400000
300000
prediction based on 2007to2009 fit
300000
400000
500000
600000
700000
NYISO.actual