INTERNATIONAL PAPER

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INTERNAL MEMORANDUM

TO: T. Saviello (Androscoggin) **DATE:** April 9, 1998

FROM: T. D. Sandry *T. D. Sandry*

SUBJECT: PM Model Verification Results -- Androscoggin B Lime Kiln PEMS Project

BACKGROUND

As part of the subject project, AN B kiln particulate matter (PM) emissions were predicted by C. Bomgardner, using six alternative neural models of measured PM, from a designed experiment conducted over August 18, to September 13, 1997. The predictions were compared to PM emission observations gathered December 16-18, 1997, during an EPA funded validation study conducted for the town of Jay, ME. The models were developed independently of the validation data, and predictions based only on operating conditions during the validation study, were supplied to the town of Jay prior to receiving the observed validation results.

Each model was compared to the observed Method 5 reference data using two statistical procedures; (1) relative accuracy test audit (RATA), and (2) continuous emission monitoring (CEM) calibration. The purpose of this comparison is to demonstrate the models performance to the mill, the town of Jay and the EPA, before deciding how to proceed with further development of PEMS models.

RESULTS

The RATA results for particulate matter (PM) were:

	Model	ES lb/hr	RM lb/hr	PEMS lb/hr	RA by RM	RA by ES	RA Used	RA Criteria	Result
1	Combo1	25	14.1	12.9	21.0	11.9	11.9	<10	FAIL
2	Combo2	25	14.1	13.2	19.3	10.9	10.9	<10	FAIL
3	PM2	25	14.1	10.0	55.9	31.6	31.6	<10	FAIL
4	PM2B	25	14.1	12.4	35.1	19.9	19.9	<10	FAIL
5	PM4C	25	14.1	12.8	26.9	15.2	15.2	<10	FAIL
6	PM4D	25	14.1	12.9	34.5	19.5	19.5	<10	FAIL

where: ES is the Emission Standard (i.e. the emission limit)
RM is the Reference Method observations averaged over the entire period
PEMS is the model predictions averaged over the entire period
RA by RM is the Relative Accuracy based on the Reference Method observations
RA by ES is the Relative Accuracy based on the Emission Standard
RA Used is based on where the RM falls relative to the ES
RA Criteria is based on where the RM falls relative to the ES
Result is whether the RA Used passes or fails relative to the RA Criteria

Details of the RATA and CEM calculation procedures are provided in the Discussion.

The neural model predictions and reference method observations are compared in Table 1 and Figures 1-6.

The CEM calibration results for particulate matter (PM) were:

	Model	Correlation Coefficient Obsvd	Correlation Coefficient Criterion	Confidence Interval, % Obsvd	Confidence Interval, % Criterion	Tolerance Interval, % Obsvd	Tolerance Interval, % Criterion	Result
1	Combo1	0.988	> 0.90	6.7	< 10	14.5*	< 25	PASS
2	Combo2	0.989	> 0.90	6.2	< 10	13.5*	< 25	PASS
3	PM2	0.953	> 0.90	13.2	< 10	27.9*	< 25	FAIL
4	PM2B	0.994	> 0.90	4.7	< 10	10.1*	< 25	PASS
5	PM4C	0.952	> 0.90	13.4	< 10	28.3*	< 25	FAIL
6	PM4D	0.911	> 0.90	18.5	< 10	38.2*	< 25	FAIL

* Since the number of samples was 12 rather than the required 15, the tolerance interval calculation is estimated by extrapolation of the table values in Appendix II - Performance Specification 11 of reference [2].

CONCLUSIONS

Although none of the models passed the RATA criteria, models Combo1 and Combo2 were sufficiently close to passing to justify using them as indicators of PM and as candidates for further improvement.

2. Two data inadequacies prevent a definite conclusion regarding the use of CEM calibration criteria to judge the validity of the models:
   - three distinct levels of particulate emissions are required, but only two were achieved during the December validation tests (see Figures 1-6), and
   - a minimum of 15 observations are required, but only 12 were obtained.

3. Three of the models, Combo1, Combo2 and PM2B, are excellant candidates for a future CEM calibration test and appear as though they would have passed, had the data been of sufficient quantity and at three distinct levels.

4. Because the models fail the RATA but appear able to pass the CEM calibration implies the models are relatively precise but inaccurate. This suggests that further investigation is needed to discover the cause.

DISCUSSION

Experimental Data and Models

A designed experiment in kiln operating variables was conducted over August 18, to September 13, 1997, at the Androscoggin B lime kiln to develop neural models of kiln response variables.

The primary response measurement was particulate matter (PM) in the stack, measured using a sampling method which is a modification of Method 5 [3]. Other responses measured and modeled included NO_x, CO, SO_2, TRS, CO_2, O_2 and Lime Availability. However, only PM is considered in this report, since it is the primary response of interest in determining how to procede with implemention of PEMS models. Neural models of each of the responses were developed by C. Bomgardner and detailed descriptions of the models and the experimental design have been posted on the Process Control Development section of the Computing & Statistics web page [4].

Subsequent to the designed experiment, a separate validation trial was run over December 16-18, 1997, for the town of Jay, ME, by Eastmount Environmental. The trial was partially funded by the EPA. The results of the trial were not used in the development of the neural models, but were only compared with the predictions from the neural models. The predictions were supplied to the town of Jay prior to receiving the validation data. The predictions from six candidate neural models and the actual observations are summarized in Table 1. The data provided by Eastmount [5] is found in Attachment 1.

Comparison of Predictions and Observations

Each model was compared to the observed Method 5 reference data using two statistical procedures; (1) relative accuracy test audit (RATA), and (2) continuous emission monitoring (CEM) calibration. The RATA procedure is a measure of the agreement of the uncorrected model predictions and the Method 5 observations, which is specified by the EPA for particulate emissions monitoring systems (PEMS) [1], such as neural models. The CEM calibration procedure is a measure of the precision of the agreement of model predictions and the Method 5 observations, after correcting the model predictions via linear calibration. The CEM calibration procedure was developed by the EPA for use with continuous in-situ PM analyzers [2], but is applied here to determine if neural models could qualify to replace CEMs in this application, due to the difficulty of the analytical measurement in a wet stack environment.

The RATA procedure

The EPA has written the RATA procedure [1] in a way that favors PEMS models that are relatively more accurate just below the emission standard, even if they are relatively less accurate when actual emissions (as measured by the reference method) are well below or just above the standard. The AN B kiln emission standard is currently 25.0 lbs/hr. I reviewed the relative accuracy calculations (see Attachment 2) and reached the following understanding of the performance specification document (see RATA definitions below).

If RMavg = or > ES, then Denom = RMavg, and RA < 20% is a pass.

If 0.25*ES < RMavg < ES, then Denom = ES, and RA < 10% is a pass.

If RMavg < 0.25*ES, then Denom = ES, and RA < 20% is a pass.

Note that only the definition of the denominator (Denom) in the RA equation (1) changes as the measured RM average values change. Also keep in mind that the confidence coefficient in the numerator is a penalty for "noisy predictions" that don't track the individual values of RM.

RATA Definitions:

RMavg is the average of the measured Reference Method values over all operating conditions

ES is the Emission Standard (currently 25.0 lbs/hr)

is the computed Relative Accuracy in %

RA = (|Dbar| + |CC|)*100% / Denom (1)

where:

= absolute value

D_i = RM_i - $PEMS_i$ is the difference between measured and predicted at observation

Dbar = (1/n)*Sum(D_i) is the average difference

CC = $t_{0.975}$ *s_D * 1/sqrt(n) is the confidence coefficient

s_D = standard deviation of the differences D (by the n-1 method)

n = number of RM measurements at the condition

= one sided student's t statistic for n-1 degrees of freedom from Table P-1 in the regulation [1].

The results of the RATA calculations are presented in Table 2 for all six models.

The CEM Calibration procedure

The EPA has written the CEM calibration procedure [2] to favor predictions which have a strong linear correlation with the RM observations and are more precise (i.e. tightly grouped) when the predicted value is at the ES, even if the slope of the calibration line is far from 1:1. In this way an analyzer which has a strong linear response, but is inaccurate (i.e. not on the 1:1 line) can be forced back onto the 1:1 line (i.e. made accurate) by calibration. I reviewed the CEM calibration calculations (see Attachment 3) and reached the following understanding of the performance specification document (see CEM calibration definitions below).

Given a set of CEM and RM data gathered according to the calibration procedure [2] which meets all the criteria for number of observarions and validity of ranges, a linear regression model is fit to the paired data with y = RM and x = CEM.

The CEM will pass the calibration test:
- If the Correlation Coefficient (equation 4) is greater than 0.90,
- and if the 95% Confidence Interval about the Mean (equation 2), evaluated at y = ES, is less than +/- 10% of ES,
- and if the Tolerance Interval for 75% of the population (equation 3), evaluated at y = ES, is less than +/- 25% of ES.

CEM Calibration Definitions:

y = RM

x = CEM

The linear regression which gives the predicted mass emission, $\hat{y}$, based on the CEM response x is given by the equation:

$$\hat{y} = m \times x + b$$

where:

$$m = \frac{S_{xy}}{S_{xx}}$$

and

$$b = \bar{y} - m \times \bar{x}$$

The mean values of the x and y data sets are given by:

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i \qquad \bar{y} = \frac{1}{n} \sum_{i=1}^{n} y_i$$

The corrected sums of squares and cross-products are given by:

$$S_{xx} = \sum_{i=1}^{n} (x_i - \bar{x})^2 \quad , S_{yy} = \sum_{i=1}^{n} (y_i - \bar{y})^2 \quad , \quad S_{xy} = \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$$

The variation of the y values around the calibration line is given by:

$$S_L = \sqrt{\frac{S_{yy}}{n-2}\left(1 - \frac{S_{xy}^2}{S_{xx} \times S_{yy}}\right)}$$

The confidence interval about the predicted value of the mean, $\hat{y}$, at the point x is given by:

$$y_c = \hat{y} \pm t_f \times S_L \sqrt{\frac{1}{n} + \frac{(x - \bar{x})^2}{S_{xx}}} \text{ with f = n - 2} \qquad (2)$$

The tolerance interval, y_T, for the regression line is given by:

$$y_T = \hat{y} \pm k_T \times S_L \qquad (3)$$

at the point x where:

$$k_T = u_{n'} \times v_f$$

and

$$n' = \frac{n}{1 + \frac{n(x - \bar{x})^2}{S_{xx}}}, n' \geq 2$$

The value of n' is truncated to the next lowest integer before looking up the value of $u_{n'}$. Values of the statistical factors, t_f, $u_{n'}$, and v_f are tabulated in Appendix II of reference [2], (see Attachment 2). Finally, the correlation coefficient may be calculated from:

$$R = m\sqrt{\frac{S_{xx}}{S_{yy}}}. \qquad (4)$$

The results of the CEM calibration calculations are presented in Table 3 for all six models.

Please call if you have any questions concerning these results or interpretations.

REFERENCES

1. Environmental Protection Agency, "Example Performance Specifications -- Example Specifications and Test Procedures for Predictive Emission Monitoring Systems", http://134.67.104.12/html/emtic/cem.htm/PEMS.WPF, January 1, 1996.

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3. Sandry, T., "Calibration of Modified Method 5 to Method 5 Androscoggin B Lime Kiln PEMS Project", Memo to T. Saviello, July 23, 1997.

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5. Laurent, M. "Final Report, Verification Test Program, International Paper Company, Androscoggin Mill", Eastmount Environmental, Inc., Project No. 97-208, January 21, 1998.

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