MODELING TRS AND SO_2 EMISSIONS FROM A KRAFT RECOVERY BOILER USING AN ARTIFICIAL NEURAL NETWORK

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ABSTRACT

A back-propagation neural network was trained to predict TRS and SO_2 emissions from kraft recovery boiler operational data. A 0.721 coefficient of correlation was achieved between actual and predicted sulfur emissions on test data withheld from network training. The ANN model found an inverse, linear relationship between TRS/SO_2 emissions and percent opacity. Disagreement between ANN model predictions on one new data set revealed conditions not present in the training data and led to the identification of an additional scenario for sulfur releases. ANN modeling offers managers a tool to analyze process variables when balancing productivity and environmental concerns.

APPLICATION

Artificial neural networks can be used to investigate recovery boiler process data. They can forecast potential upsets and help reveal underlying causes.

EXECUTIVE SUMMARY

Artificial neural networks have proven to be useful tools for modeling complex processes where classical approaches often fall short. This paper discusses the use of a back-propagation neural network to create a model of TRS and SO_2 emissions from kraft recovery boiler operational data. Good correlation was achieved between actual and predicted sulfur emissions on test data withheld from the network during its training. The ANN model disclosed several relationships between process variables and sulfur emissions. Three of these relationships, percent oxygen in the flue gas, black liquor loading and percent opacity are discussed in this paper.

The ANN model disclosed the inverse relationship between the percentage of oxygen remaining in the flue gas and TRS/SO_2 stack emissions. Boiler loading, indicated by black liquor flow, was directly related to the amount of sulfur emitted to the atmosphere. The network also revealed an inverse, linear relationship between TRS/SO_2 emissions and percent opacity.

Of particular interest is the ANN model=s interpretation of one set of new boiler data. Disagreement between the ANN model=s predictions revealed a set of conditions that was not well represented within the training data set. This led to the identification of an additional scenario for sulfur releases. In this case the ANN model proved to be a helpful diagnostic tool for analyzing process variables when balancing productivity and environmental concerns.

INTRODUCTION

This paper demonstrates how artificial neural network (ANN) modeling can reveal the relationships among process variables, boiler productivity and sulfur emissions within a kraft recovery boiler. A broader understanding of the link between boiler variables and sulfur emissions would be helpful to kraft paper mills worldwide. The release of sulfur from the recovery boiler stack is a two-fold economic problem. First, any sulfur losses must be replaced with the purchase of additional sodium sulfate. Second, the emission of sulfur to the atmosphere is an environmental problem that poses a legal liability, generates poor community relations and may be subject to emission tonnage fees.

Artificial neural networks and neurocontrol strategies are rapidly gaining the attention of researchers in the pulp and paper industry (1-5). With appropriate software, neural techniques can transform routine process data into a sophisticated model. Because ANN=s are based strictly on data rather than on assumptions, neural-derived models have an uncanny ability to predict site- and equipment-specific outcomes. At the same time, as they sift through complex, noisy or imprecise data, they can reveal underlying quantitative and phase relationships among the input variables. Neural network models usually outperform traditional mathematical models of coupled nonlinear and differential equations.

Artificial neural networks are ideal tools for process simulation because they require no initial assumptions or simplifications to the physical and chemical principles that ultimately define the process. Furthermore, ANNs allow for continuous refinement of the simulation as equipment ages, processes are modified, or starting materials vary. Several pulp and paper process areas have already been examined with neural techniques. Qian *et al.* (1) modeled a wood-chip refiner to optimize pulp yield and strength. Miyanishi and Shimada (2) diagnosed web breaks on newsprint paper machines. Milosavljevic and Heikkila (3) evaluated the efficiency of heat recovery in dryer hood scrubbers of paper machines. Rumph and Rudd (4) and Baines *et al.* (5) advanced design guidelines for replacing continuous emission monitoring systems (CEMS) in the pulp and paper industry with neural-based predictive emission monitoring systems (PEMS).

The complexity associated with recovery boiler combustion processes has hindered the creation of an all-encompassing model. Further complicating the creation of a detailed recovery boiler model is the fact that each unit has its own nuances and the chemical composition of black liquor varies among kraft mills. Despite these inherent problems, several mathematical models have been advanced for various components of the kraft recovery process. Grace *et al*. (6), for example, developed a computational fluid dynamics model that predicts some relationships between droplet size, gas flow patterns, oxygen concentrations, and black liquor combustion. Verril and Wessel (7) created a model for sodium release during black liquor droplet combustion. Walsh *et al*. (8) utilized the computational fluid dynamic models created by Karvinen *et al*. and Grace *et al*. (6) to determine the most efficient way to increase combustion efficiency with additional boiler air supply. Wag *et al*. (9) developed a model predicting the release of carbon, sodium, potassium, chloride, and sulfur during char burning. A three-dimensional model created by Wessel *et al*. (10) improved predictions of turbulent flow, combustion, and heat transfer by considering black liquor combustion as droplets and as deposits on furnace walls. None of the models above addresses the environmental concern of sulfur emissions from kraft recover boilers. Our earlier research attempts involved the use of ANN modeling to lower TRS emissions and alleviate sulfur odors emanating from the mill (11). To our knowledge, our research group is the first to utilize neural techniques to gain new insights about sulfur losses from recovery boilers.

RECOVERY BOILER VARIABLES

Sulfur can escape a kraft boiler in three general forms. The first is volatile total reduced sulfur compounds (TRS), *e.g.*, hydrogen sulfide, dimethyl sulfide, dimethyl disulfide, and methyl mercaptan. These compounds are notorious for their strong, objectionable odors. A second form is gaseous SO_2. Sulfur dioxide has a less offensive odor, but is a lung irritant and contributes to acid deposition. The third form is solid sodium sulfate, the primary chemical in the particulate emitted by the recovery boiler, but reusable if recovered. Of the three forms of sulfur that can leave the boiler, the easiest to control (via electrostatic precipitators) is the sodium sulfate. The ANN model was created to optimize the boiler operating parameters in order to reduce TRS and SO_2 emissions from the stack, while not compromising overall boiler productivity. TRS and SO_2 were summed into a single value representing undesirable sulfur losses and termed total sulfur (TSUL).

Five categories of boiler parameters under operator control, either directly or indirectly, were used as inputs to the neural network (**Table 1**): liquor, air flow/pressure, furnace draft, particulate emissions and boiler productivity. A rationale for the inclusion of each category is detailed below.

Liquor variables influence the size of the droplets formed when the black liquor is sprayed into the boiler. Black liquor flow, spray gun nozzle pressure, liquor temperature, liquor percent solids and saltcake addition rate were obvious choices for network inputs. Droplet size and percent solids influence particle entrainment, as well as the drying, devolatilization, swelling and char burning characteristics of the liquor. Black liquor flow indicates boiler loading.

Air flow/pressure parameters dictate the amount of oxygen entering the boiler and control combustion efficiency. Primary, secondary and tertiary windbox pressures and flows were included as ANN inputs. Windbox pressures relate to the force with which the air enters the boiler. Primary and secondary air are preheated in order to enhance boiler efficiency by preventing cool air from entering the hottest zones of the boiler. Damper positions influence both airflow and pressure. Primary air also shapes the char bed forming on the furnace floor. The shape of the bed influences sulfate reduction efficiency and fuming (12). Primary air is also responsible for supplying oxygen to the char bed. Too little oxygen at the bed surface will result in a low bed temperature and a heterogeneous temperature distribution, causing insufficient sulfate reduction and excess fuming (13). Secondary airflow provides more oxygen, and its introduction velocity aids in the mixing of boiler gases. Tertiary airflow adds the last infusion of oxygen into the flue gas.

Abbreviation	**Parameter Description**	**Unit of Measure**	**Low Value**	**High Value**
TSUL	Total Sulfur (TRS + SO_2)	ppm	5.7	209.3
LIQF	Black Liquor Flow	gpm *(L/s)*	249.9 *(15.76)*	282.5 *(17.82)*
NOZP	Liquor Gun Nozzle Pressure	psi *(kPa)*	30.9 *(213)*	36.1 *(249)*
LIQT	Black Liquor Temperature	degrees F *(K)*	211.7 *(373.0)*	219.6 *(377.4)*
DENS	Black Liquor Solids	percent	61.94	67.27
SRPM	Saltcake Addition Rate	rpm	9	14
PAFL	Primary Air Flow	10^3*lbs/hour *(kg/s)*	176.1 *(22.19)*	207.8 *(26.18)*
SAFL	Secondary Air Flow	10^3*lbs/hour *(kg/s)*	227.4 *(28.65)*	318.2 *(40.09)*
TAFL	Tertiary Air Flow	10^3*lbs/hour *(kg/s)*	78.1 *(9.84)*	95.0 *(12.0)*
PAIR	Primary Air Damper Position	% open	49.9	58.1
SAIR	Secondary Air Damper Position	% open	49.0	69.0
TAIR	Tertiary Air Damper Position	% open	43.9	53.2
PWB	Primary Windbox Pressure	in. of H_2O *(m)*	1.47 *(0.0373)*	2.79 *(0.0709)*
SWB	Secondary Windbox Pressure	in. of H_2O *(m)*	5.17 *(0.131)*	13.65 *(0.3467)*
TWBa	Tertiary Windbox A Pressure	in. of H_2O *(m)*	10.59 *(0.2690)*	16.88 *(0.4288)*
TWBb	Tertiary Windbox B Pressure	in. of H_2O *(m)*	11 *(0.28)*	17 *(0.43)*
PAT	Primary Air Temperature	degrees F *(K)*	274 *(408)*	320 *(433)*
SAT	Secondary Air Temperature	degrees F *(K)*	298 *(421)*	303 *(424)*
DRFT	Furnace Draft	in. of H_2O *(m)*	-0.32 (-8.2^{-3})	-0.19 (-4.8^{-3})
FNSP	Induced Draft Fan Speed	rpm	250	334
O2	Oxygen in Flue Gas	percent	1.1	3.4
OPAC	Opacity	percent	5.5	30
STFL	Steamflow	10^3*lbs/hour *(kg/s)*	227 *(28.6)*	509 *(64.1)*
SPHO	Superheater Temperature	degrees F *(K)*	663 *(624)*	753 *(674)*
PPTT	Electrostatic Precipitator Temperature	degrees F *(K)*	405 *(480)*	465 *(514)*

** SI units and values are shown in parenthesis where applicable.*

Table 1. Recovery Boiler Input-Output Values.

Furnace draft parameters characterize internal gas velocity and are also indicative of smooth boiler operation. Furnace draft, induced draft fan speed and percent oxygen comprised this input group. A sudden increase in furnace draft or induced draft fan speed might suggest plugging due to hot entrained particles adhering to heat exchanger tubing. Percent oxygen in the flue exhaust was also used to register the boiler=s operating conditions. Too little oxygen in the flue gas may indicate incomplete combustion, while an excessively high percentage could testify to poor mixing conditions.

Percent opacity was included as an input variable since it tracks escaping sulfate particulates. Complete oxidation of reduced sulfur compounds present in the upper furnace would lead to an increase in sodium sulfate particulate in the stack gas. This increase would lead to more particulate entering the precipitator and could cause higher opacities.

Boiler productivity was described by steam production, superheater temperature and electrostatic precipitator temperature. Superheater temperature is correlated with boiler operating temperature and particle entrainment. To maintain good heat transfer, the superheater must be free from significant fume deposits and be exposed to adequate flue gas temperatures. The temperature within the precipitator was also used to show boiler efficiency by providing an indication of how much heat was lost to the flue gas.

The list of variables presented in Table 1 is a refinement of the original set employed. Other parameters demonstrated no forecast value in earlier trials; these parameters were systematically pruned from the network as it underwent development. Some potentially useful parameters, such as droplet size and internal boiler temperature distribution, remain unknown. Their role was indirectly accounted for by the inclusion of parameters known to influence them.

EXPERIMENTAL METHODS

Neural networks require large amounts of data for training. The effort required to enter process variables by hand is impractical. The recovery boiler we studied was the only unit interfaced to a comprehensive data acquisition system (DAS). In addition it was the largest recovery boiler and the object of local environmental scrutiny. New source performance standards (NSPS) required that boiler operating parameters and stack emissions are continuously recorded as 6-minute averages. These data were downloaded from the DAS and input to a neural network. All neural network activities were performed with Version 3.11 of the BrainMaker Professional software (California Scientific Software, Nevada City, CA, USA) and Version 3.1 of its accompanying neural network spreadsheet NetMaker. The sections below assume some familiarity with ANN theory and application. Two excellent introductions to ANN use in pulp and paper industry have previously appeared in this journal (References 1 and 3).

We performed substantial manipulations on the data before it was imported into the neural network software. A historical time series was created for each input variable so that a training fact contained the current value plus a 30-minute history (the five previous 6-minute interval values). This process resulted in 144 input neurons. Actual network construction required the deletion of spurious/missing values during periods of sensor calibration or sensor malfunction. Since a spurious/missing value would appear in the 30-minute history for the next five facts, a total of six facts had to be expunged on each occurrence. Input parameters were normalized to generally fall within a range between 10 and 99. This was done to prevent the network from over-emphasizing variables with high absolute values and ignoring those with fractional absolute values.

The architecture of the ANN was refined to produce the best overall testing results. The final network had two hidden layers with 86 neurons in the first hidden layer and 53 in the second. The sole output neuron was total sulfur (TSUL) in parts per million. A total of 1473 facts were compiled from six different 48-hour periods (3/6-3/7/98, 3/14-3/15/98, 6/21-6/22/98, 9/20-9/21/98, 10/14-10/15/98, and 10/17-10/18/98). Training was performed using 90% of the facts; 10% (147 facts) were withheld from training and used for testing. A linear learning rate of 0.80 was selected to reduce the size of the changes made to the weighting factors. Tolerance tuning initially set at 0.4 of the TSUL range was also employed. Tolerances were successively reduced until network learning stalled or a minimum tolerance of 0.1 was achieved. A noise value of 0.05 was added to the training data to help the network generalize rather than memorize the relationships among variables.

RESULTS AND DISCUSSION

Predicted and actual TSUL values are plotted in **Figure 1** for the test facts from the network described above. The network successfully trained and tested to a 0.16 tolerance level after 2000 iterations. The chosen variables for the ANN model are good predictors of the boiler=s total sulfur emissions as demonstrated by the broad dynamic range displayed by the output neuron. The ANN was trained over a large range of TSUL values (5.7 - 209.3). This helped to ensure that the network had Aseen≅ the output for many types of anticipated boiler conditions. This is necessary because the trained network can only choose output values that fall within the training range.

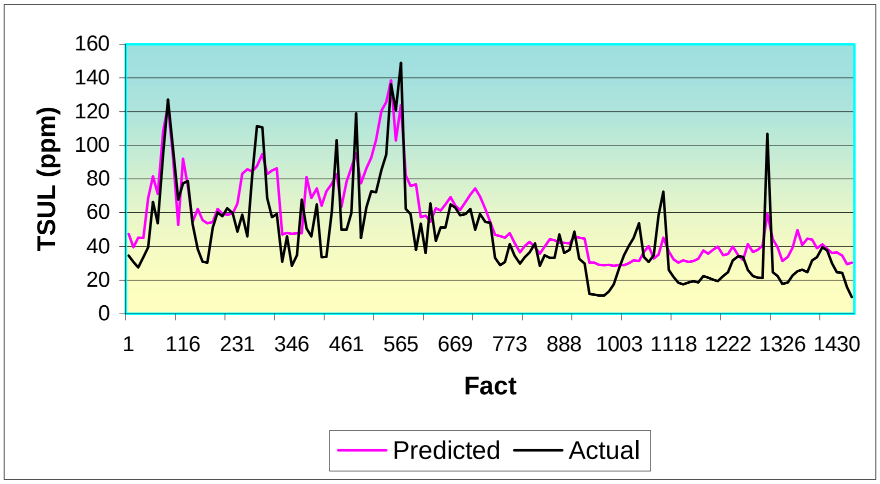

Figure 1. Predicted and actual total sulfur emissions for withheld test data.

Figure 2 correlates the actual *versus* predicted TSUL for the test data. The plot indicates that the network can predict TSUL over the entire range of training values with equal success. Random, homoscedastic scatter is responsible for the R^2 value of 0.721. Equal distributions of points both above and below the line support the use of a linear relationship. The resulting line through the points has a slope slightly less than one, which means the network generally underpredicts the resulting TSUL output.

The trained network was analyzed to determine which input neurons were most important in predicting TSUL. Initially, each input neuron was varied by +/- 10% of its range while all other inputs were held constant. This was done for every neuron and fact in the set of training data. The resulting values were paired with the average response of the output neuron (change in TSUL with +10% input neuron variation plus change in TSUL with B10% variation divided by 2). This produced a ranking of the input neuron sensitivity from those with the largest positive effect on the TSUL output, to those with the largest negative effect. The input neurons with the strongest influence over the TSUL output, both directly and inversely, were then re-examined to display the type of relationship each of the selected inputs would have on the output neuron. Figures 3 and 4 are the ANN=s representation of the relationships found between TSUL and two input variables, $\%O_2$ and liquor flow.

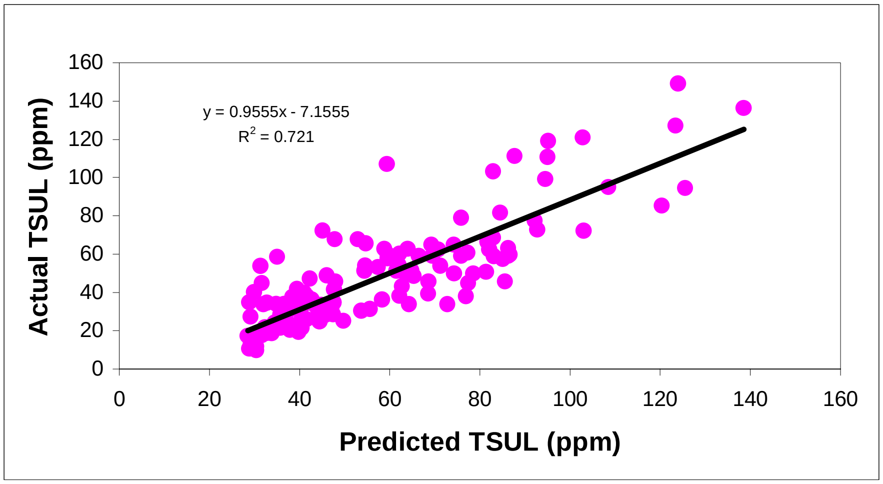

Figure 2. Correlation plot between actual and predicted TSUL.

The % O_2 remaining in the stack gas has a direct bearing on the TSUL output (**Figure 3**). Combustion engineers are well aware of this relationship; the fact that the network model found it without prompting gives the modeling technique a level of validation. Clearly, when the % O_2 in the exhaust gas is low, the level of excess oxygen is insufficient to complete the oxidation of sulfur species to sulfate (S +6). This produces low opacity and a high concentration of sulfur dioxide (S +4) and TRS (S B2) in the stack emissions. The % O_2 trace is non-linear, so TSUL emissions increase exponentially as oxygen levels decrease.

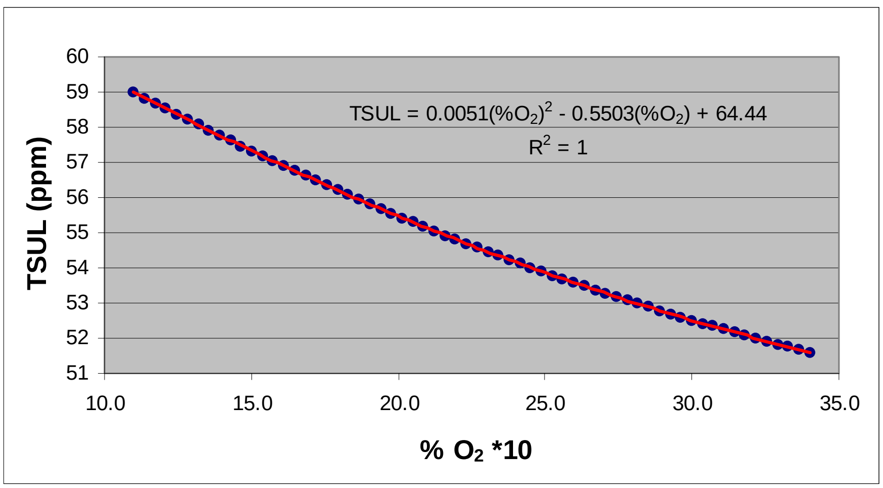

Figure 3. The relationship between TSUL and %O_2 extracted from the trained ANN.

As black liquor loading to the boiler increases, so do the overall stack emissions (**Figure 4**). This relationship makes intuitive sense, since higher liquor loads tax the combustion process for adequate gas mixing, lower the percentage of oxygen available and increase the quantity of sulfur within the boiler. Its nonlinear character indicates that problems could quickly worsen under higher black liquor flow.

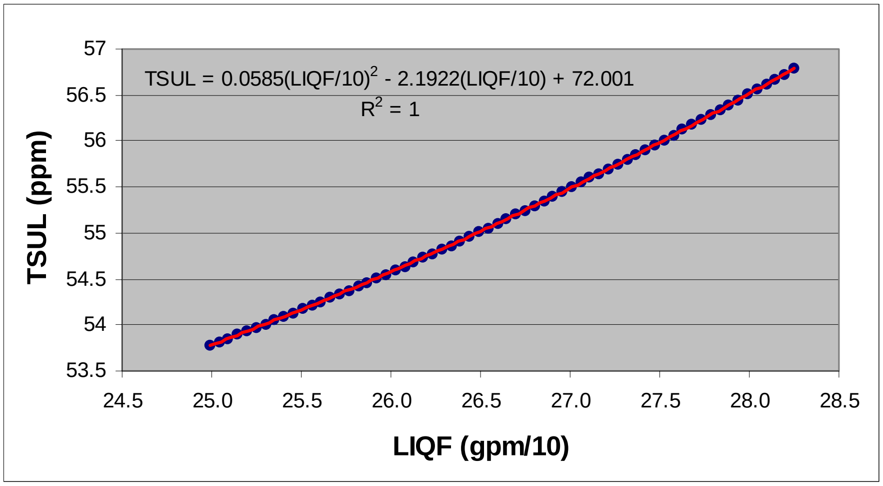

Figure 4. The relationship between liquor flow and TSUL extracted from the network.

The partitioning of sulfur between the completely oxidized sulfate form and incompletely oxidized TSUL forms is shown in **Figure 5**. Since % opacity is dominated by sulfate particulate, it is a good indicator of sulfate levels. When sulfate levels are high, there is a corresponding reduction in TSUL. When TSUL is high, the % opacity is low. The relationship is quite linear (R^2 = 0.9996), suggesting a simple, inverse proportionality.

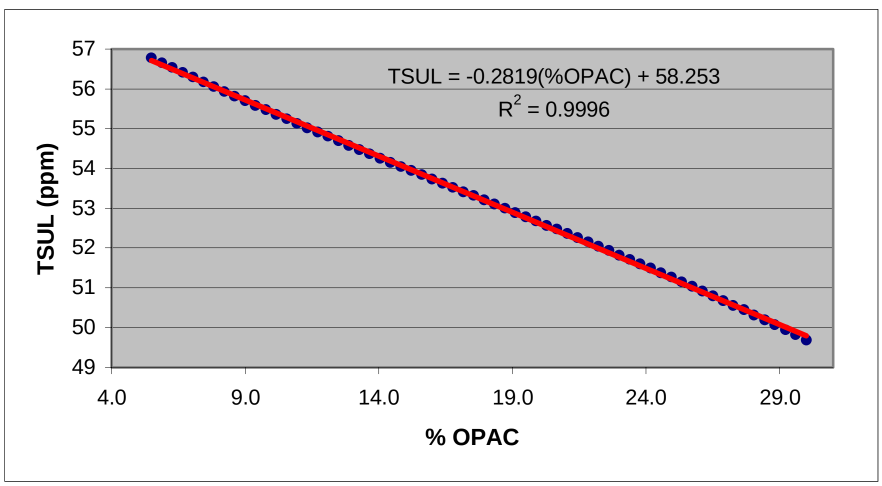

Figure 5. The relationship between TSUL and % opacity extracted from the network.

Figures 3 and 4 indicate that many relationships in the ANN are non-linear. These complex relationships are often not adequately represented using multiple regression techniques. Correct use of regression procedures requires advanced knowledge of the form of the underlying relationship (e.g., linear, exponential, logarithmic, etc.). Even with an ANN to help uncover the appropriate model for each input variable, regression techniques still proved inadequate. While it is not difficult to elucidate the general effect each input neuron has on the output of the network, it is quite difficult to use these resulting relationships to create a simplified model. The ANN responds far better to the complexity of the interrelated variables than any regression model we extracted from the trained network.

The value of a model can be demonstrated in what it reveals when applied to new, unknown data. Model shortfalls can often prove more instructive and interesting than the successes. **Figure 6** shows the network=s predictions of total sulfur loss on one particular set of boiler data that was not used in its training. The ANN reasonably forecasted the sulfur loss for much of the period, but clearly failed to predict the large excursion between facts 150 and 200.

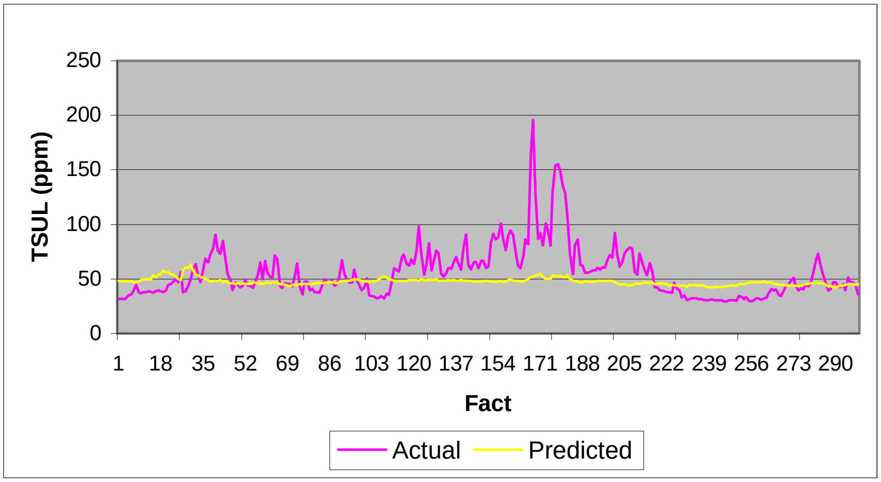

Figure 6. Resulting TSUL predictions from the trained network on a new set of data.

Failure of the model was prompted by boiler conditions that were not encompassed in the training set. The ANN model interpreted the input parameters in the unseen data set and determined that during this period of time the boiler should be operating smoothly with little change in the TSUL emissions. For most of the unseen data, this is true. But between facts 150 and 200, the TSUL emissions show two dramatic spikes. In order to understand what caused the model to break down, the raw data were re-examined.

The large TSUL emissions correspond to a period of high boiler loading (black liquor flow) and very low levels of excess oxygen in the flue gas **(Figures 7** and **8**). This example demonstrates one weakness of the neural network model. It can only predict the outcome for situations for which it has seen adequate repetitions. While the network learned the correct relationship between these inputs and the output neuron, only a few examples of these conditions were in its training base. Since the network had not learned this relationship to the degree presented in the new data set, it responded too weakly to the causes for the spikes. The network predicted only the very small increases in TSUL visible in the predicted trace immediately underneath the two spikes. Inclusion of this unseen data to the training basis for the network should yield improved performance under similar circumstances in future data sets.

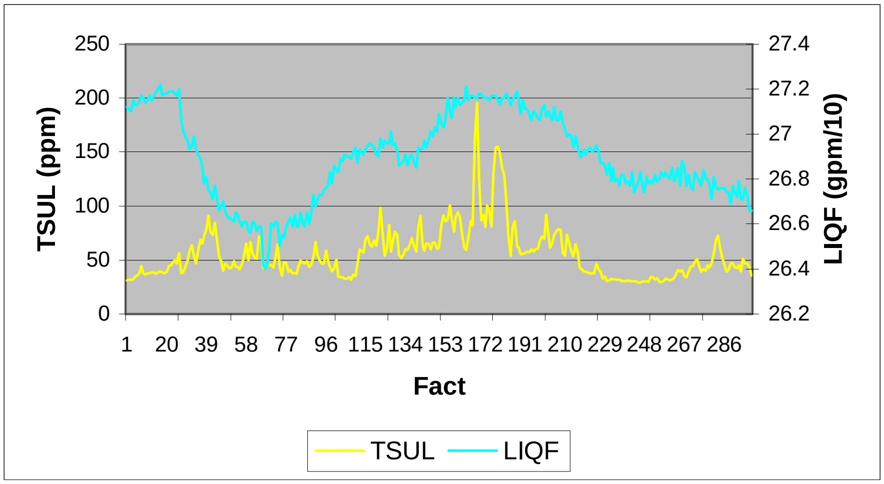

Figure 7. Liquor flow and TSUL emissions for the new data set.

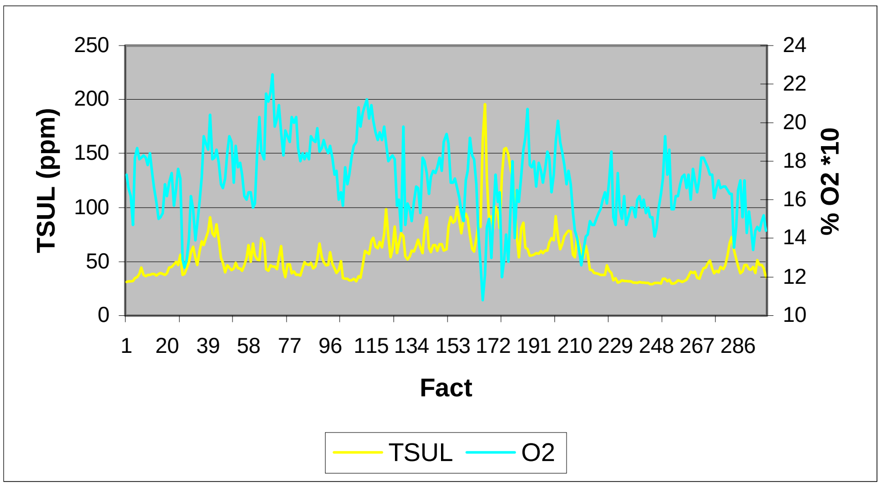

Figure 8. Percent O_2 and TSUL emissions for the new data set.

CONCLUSIONS

ANN techniques offer a viable method for modeling the complex nature of kraft recovery boiler emissions. This ANN model was substantiated by its confirmation of accepted boiler physical and chemical processes. Run in a real-time application, it could help assure an operator or foreman that the unit is operating in a predictable fashion. Discrepancies between the predictions of a well-established ANN model and the current boiler performance indicate unusual unit behavior has occurred. An examination of the incongruous data with the trained network can be a useful tool for assessing underlying causes and providing guidance for avoiding excess emissions. Furthermore, the network can be periodically updated by the inclusion of new data sets into its training basis. This allows for parameter evolution such as equipment aging or changes in black liquor composition. A revised network can help formulate a new operational procedure for the minimization of TRS and SO_2 emissions, while maintaining desired green liquor and steam production.

We believe several important additions to the set of input neurons could lead to the creation of an improved ANN model. These data were not available for the boiler we studied. The inclusion of actual or calculated black liquor droplet sizes should lead to better TSUL predictions. Temperature distributions and internal gas flow patterns would also be useful in forecasting TSUL emissions. While these parameters are difficult to measure, theoretical constructs can be employed to calculate their values for use as input neurons. Our future efforts will blend ANN and traditional modeling techniques to improve our ability to accurately predict outcomes of highly complex processes.

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