

NEURAL NETWORK PREDICTIVE PROCESS MODELS: THREE DIVERSE MANUFACTURING APPLICATIONS

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Introduction to Neural Network Predictive Process Models

In a broad sense, predictive models describe the functional relationship between input and output variables of a data set. When dealing with real world manufacturing applications, it is usually not an easy task to precisely define the set of input variables that potentially affect the output variables for a particular process. Often times, this is further complicated by the existence of interactions between the variables. Even if these variables can be identified, finding an analytical expression of the relationship may not always be possible. The process of selecting the analytical expression and estimating the parameters of the selected expression could be very time consuming.

Neural networks, a field which began approximately 50 years ago, has been getting more attention over the past 15 years. There are a number of survey papers that summarize some of the applications of neural networks [Udo, 1992, Zhang and Huang, 1995, Hussain, 1999]. The first one surveys within the manufacturing domain, which covers resource allocation, scheduling, process control, robotic control and quality control. The second one provides a good overview of many manufacturing applications. The final one discusses a variety of applications in chemical process control. One of the advantages of neural network modeling is its ability to learn relationships through the data itself rather than assuming the functional form of the relationship. A neural network is known as a universal approximator [Hornik et al., 1989, Funahashi, 1989]. It can model any relationship to any degree of accuracy given that there is

sufficient data for modeling. It can tolerate noisy and incomplete data representations. Moreover, it can dynamically adjust to new process conditions by continuous training. Through an iterative learning process, neural network extracts information from the training set and stores the information in its weight connections. After a network is trained, it can then be used to provide predictions for new inputs. But how good is the network when it is used to make predictions on data that is not used to train the network?

Being an empirical modeling technique, validating the network is at least as important as constructing the network. Theoretically speaking, an infinite number of data points should be used to validate and evaluate the performance of a network. However, this is not practically feasible to do. In order to maximally leverage the available data, resampling methods such as **cross validation** and **group cross validation** can be used to validate the network [Twomey et al., 1995, Lam et al., forthcoming, Lam and Smith, 1998, Coit et al., 1998]. These validation methods are more appealing than the traditional **data splitting** approach, especially when the data is sparse. They allow the construction of the network based upon the entire data set but also allow the evaluation of the network using all the data that is available [Efron, 1982, Wolpert, 1993]. Hence, these methods ensure the extraction of as much information from the available data as possible for developing an **application network**, ensuring the best possible prediction performance. The trade off of using these resampling methods is the incurred computational expense of developing multiple **validation networks** in order to infer the performance of the application network [Twomey and Smith, 1998].

This chapter discusses some applications where neural networks have been used successfully as predictive process models. These applications have relatively sparse data sets, therefore resampling methods are used to validate the application networks. More specifically,

the manufacturing processes covered include: (1) a ceramic slip casting process, (2) an abrasive flow machining process, and (3) a chemical oxidation process. These examples are real world engineering problems where designed experiments were conducted for the first and the last examples to supplement production data.

Ceramic Slip Casting Application

The slip-casting process is used to produce ceramic ware in many complicated shapes such as bowls, statues and sinks that cannot be achieved through conventional pressing. However, this flexibility does not come without a price. It is generally more difficult to achieve a desired level of product quality in the presence of many controllable and uncontrollable process factors. Basically, the manufacturing of ceramic ware consists of the following steps:

1. preparing the liquid clay (a slurry, or slip);
2. casting the slip in a plaster mold for a specified duration;
3. removing the mold;
4. air drying the cast piece;
5. spray gazing the dried piece;
6. firing the gazed piece in a kiln; and
7. inspecting the finished product.

The slip is prepared by mixing clay powder with a suspending liquid. Deflocculants are added to the slurry to provide stability and density, and binders are added to ensure that the resulting cast is strong enough to be handled. This slip is then poured into a plaster mold and stays there for a specified time period in order to form a solid product. The liquid in the slip is absorbed into the mold through capillary action, resulting in a solid cast inside the mold. When it is estimated (by the slip cast operators) that the cast has reached the desired wall thickness, it is then removed

from the mold, air dried, glazed, and fired to produce a finished product [Adams, 1988]. Slip casting largely determines the quality of the final product. If the slip casting process takes too long, the cast will be too dry and may result in cracks. On the other hand, if it does not allow sufficient time period for the slip to cast, the cast piece will be too wet and may result in instabilities. These defects are manifest in the subsequent steps of the manufacturing process. Defects that are found before the ware is fired can often be repaired. For defects that cannot be repaired, the material can be recovered, but the considerable labor and overhead are still irretrievably lost. Most defects that are found after firing result in a complete loss of the defective piece. The proportion of defective pieces due to casting imperfections can approach as much as 30%. This figure obviously poses a significant problem that affects the efficiency and profitability of these manufacturing firms.

The primary causal factor for cast fractures and/or deformities is the distribution of moisture content inside the cast before firing. When the moisture differential, or *moisture gradient*, inside the wall of the cast is too steep, it results in stress differences. It is the stress differences that cause the piece to deform and eventually fracture. In order to minimize the possibility of fractures or deformities, the moisture content should be as uniform as possible. In other words, the moisture gradient should be close to zero in order to have a good cast. Another important measure is *cast rate*, which is actually the thickness of the cast (in inches) achieved during a set time in the mold. A larger cast rate is more desirable because it indicates an increase in production efficiency.

The quality of the cast (moisture gradient) and the cast rate depend on the slip conditions, the ambient conditions in the plant, and the plaster mold conditions. As the age of the mold increases, the capillary action of the mold degrades, which causes an increase in the required

casting time. Ambient conditions also have a significant effect on casting time. Molds that are cast under hot, dry conditions (i.e., near a kiln) require less casting time than molds cast under cooler, wetter conditions (i.e., near the building exterior). The variance of ambient conditions across the plant can be a significant problem in ceramic casting facilities. Two ambient variables (the plant temperature and humidity), ten slip property variables, and the cast time are identified as significant factors for determining the cast quality and the cast efficiency. These variables are summarized in Table 1.

Insert Table 1 here

Neural Network Modeling for Slip Casting Process

Two separate networks were developed where one of them was used to predict the moisture gradient and the other one was constructed to predict the cast rate. The dual models' approach was motivated partly because of the uneven distribution of the data. However, the main motivation behind this was the undefined underlying relationship between the process variables and the unknown interactive behavior of the variables.

Two separate data sets (consisting of production data supplemented by experimental data) were collected and obtained by the plant technicians. There were 367 observations for the moisture gradient model and 952 observations for the cast rate model. Both of these models have the same set of input variables as illustrated in Table 1. The network architectures, training parameters and stopping criteria were finalized through experimentation and examination of preliminary networks. An ordinary backpropagation algorithm was used because of its simplicity and its documented ability as a continuous function approximator [Hornik et al., 1989,

Funahashi, 1989]. The final application network architecture for the moisture gradient model had 13 inputs, two hidden layers with 27 hidden units in each layer, and a single output. The output unit represents the moisture gradient of the cast piece. Similarly, the architecture for cast rate model had the same input variables, two hidden layers with 11 hidden units in each layer, and a single output which represents the cast rate of the slip casting process.

In order to assure that the plant engineers and supervisors have faith in the models, and that the neural network predictions were accurate, a five-fold group cross validation method was used to validate the two application networks. This resampling method allows all the data to be used for both construction and validation of the neural network prediction models. This approach divided the available data into five mutually exclusive groups. Five validation networks were constructed, using the same parameters as the application network described above, where each used four groups of data to train the validation network and test it on the hold back group. Each validation network had a different hold back group as a test set. The errors of the five test tests provide an estimate of the generalization ability of the application network.

Tables 2 and 3 summarize the mean absolute errors (MAE) and root mean squared errors (RMSE) of the validation and application networks for the moisture gradient network and the cast rate network. Typically, the error measures on the validation networks are not as good as that on the application network. This observation is obvious because the errors of the application network were calculated by resubstituting the training data back into the model whereas the errors of the validation networks were obtained using the five hold back test sets.

Insert Tables 2 and 3 here

Figure 1 shows typical cross validation network predictions for the moisture gradient network and Figure 2 shows a similar graph for the cast rate network. By comparing these figures, it appears that the cast rate network performs better than the moisture gradient network. The predictions of the cast rate application network are accurate over the entire range of the process variables. On the other hand, the predictions of the moisture gradient network are fairly accurate, except for large values of the target. This can be explained by the skewed distribution of the data (367 observations) where almost ninety percent of the data have values of moisture gradient less than 0.01 (see Figure 3). Also, there was considerable human error possible in the moisture gradient measurement. However, despite the imperfection of the performance of the moisture gradient network, it provides adequate precision for use in the manufacturing plant.

Insert Figures 1, 2 and 3 here

Abrasive Flow Machining Application

Abrasive flow machining (AFM) was originally developed for deburring aircraft valve bodies. It has many applications in the aerospace, automotive, electronic and die-making industries. The product spectrum includes turbine engines, fuel injector nozzles, combustion liners and aluminum extrusion dies. It is a special finishing process that is used to deburr, polish or radius surfaces of critical components. However, it is not a mass material removal process. AFM removes small quantities of material by a viscous, abrasive laden semi-solid grinding media flowing under pressure through or across a workpiece. The AFM process acts in a manner similar to grinding or lapping where the extruded abrasive media gently hones edges and surfaces. The abrasive action occurs only in areas where the media flow is restricted. The

passageways that have the greatest restriction will experience the largest grinding forces and the highest deburring ability.

AFM can process many selected passages on a single workpiece or multiple parts simultaneously. Generally, the media is extruded through or over the workpiece with motion, usually in both directions. It is particularly useful when applied to workpieces containing internal passageways that are inaccessible using conventional deburring and polishing tools [Rhoades, 1991]. However, AFM has not been widely used because of the lack of theoretic support for the complex behavior of the process. In order to understand the process, a large range of process parameters such as extrusion pressure, media viscosity, media rheology, abrasive size and type, and part geometry must be taken into consideration.

Engine Manifolds

An air intake manifold is a part of automotive engines (see Figure 4), consisting of 12 cylindrical “runners,” (the shaded parts in Figure 4) through which air flows. These runners have complex geometries. The manifold is attached to the throttle body in the engine through a large hole (middle front of Figure 4). Engine manifolds are typically sand cast aluminum and are too complex to be economically machined by conventional methods. The sand cast cavities have rough and irregular surfaces that retard air flow, particularly at the passage walls. This imperfect finish has a significant detrimental impact on the performance, fuel efficiency, and emissions of automotive engines [Smith, 1997].

Insert Figure 4 here

AFM can finish sand cast manifolds so that the interior passages are smoother, more uniform and can achieve more precise air flow specifications. This can increase engine horsepower and improve vehicle performance. However, the AFM process is not currently economical for mass production of manifolds. Currently, in order to AFM engine manifolds, technicians preset values for the volume of media that will be extruded through the manifold and the hydraulic extrusion pressure based on their judgment and experience. After this operation is finished, they clean the manifold, air dry the part and test the outgoing air flow. If specifications have not been made, they will repeat the process until the manifold achieves the desired air flow requirements. On the other hand, if the manifold is overmachined, the part is scrapped.

Process Variables

The outgoing air flow rate (the air flow rate achieved after the AFM process) of an engine manifold depends on the part characteristics, the AFM machine settings, the media conditions and the ambient conditions in the plant. These process variables are categorized as follows:

1. Incoming part characteristics:
 - weight;
 - surface roughness inside the throttle body orifice;
 - air flow rate through each paired runner;
 - variability of the air flow rate among the six pairs of runners;
 - diameter of the throttle body orifice.
2. AFM machine settings:
 - volume of media extruded through the manifold;
 - hydraulic extrusion pressure;
 - media flow rate through the manifold;

- number of cycles of the AFM machine piston.

3. Media conditions:

- temperature of the media;
- temperature of the manifold;
- number of parts machined prior to the current part in a work day;
- sequence of production during the day.

There is considerable variability among the shipped manifolds due to the limitations of the sand casting process. The volume of media extruded and the extrusion pressure are preset by the operator depending on his judgment of when the manifold reaches air flow specifications. These two machine settings determine the number of cycles needed and the media flow rate for the process. Media condition is extremely important because it relates to the cutting ability of the media. The media starts new with an amount of abrasive grit and no impurities. Over time, impurities enter into the media from the metal being machined and the grit becomes less abrasive and contaminated. This has a profound impact on the AFM process. However, measurement of media condition during processing is impossible. Another change in media condition occurs daily because the behavior of the media depends partially on its temperature. At the beginning of a day, the media is cold and a relatively higher machining ability can be achieved. However, after repeated processing, it becomes heated and hence lowers the AFM ability. The sequence of production and the number of parts machined prior to the current part are very crude approximations to this heating effect. Time of production was divided into five periods beginning in the morning (period 1) and ending with the work day (period 5). Each part was assigned to one of these periods depending on its time of production. The number of parts

machined prior to the current part is simply a counter for another measure of the changing characteristics of the media during a work day.

Neural Network Modeling for Abrasive Flow Machining Process

Production data was collected and after processing, 58 observations were left for analysis. The data set consisted of static information as well as dynamic information. The extrusion pressure, volume of media extruded, media flow rate and media temperature were collected on a per cycle basis during the machining process. These dynamic process variables were used to derive the statistics median, average, gradient, range and standard deviation. Using these additional variables along with the static information, a first order stepwise regression model was constructed to predict the outgoing average air flow rate of the manifolds. The critical process variables are as follows:

- average air flow rate before AFM;
- average hydraulic extrusion pressure;
- median of media flow rate;
- range of media temperature;
- range of part temperature;
- standard deviation of volume of media extruded;
- number of parts machined prior to the current part.

Regression results showed that these seven process variables can explain 87.00% of the variance of the outgoing average air flow rate. These variables were then used as inputs to the neural network. A static neural network model was developed in favor of a dynamic one because it is simpler to construct and to operate.

The neural network for predicting the outgoing average air flow rate of the engine manifolds was created using the cascade-correlation paradigm. A cascade-correlation learning algorithm was used because it learns very quickly and the network determines its own topology and its own size [Fahlman and Lebiere, 1990]. This algorithm begins with no hidden neurons, with only direct connections from the input units to the output units. Then, hidden neurons are added one at a time. The purpose of each new hidden neuron is to predict the current remaining output error in the network. Unlike the traditional backpropagation learning algorithm, hidden neurons are allowed to have connections from the pre-existing hidden neurons along with connections from the input units. Figure 5 illustrates a typical cascade architecture.

Insert Figure 5 here

The training parameters and the maximum number of epochs were selected through experimentation and examination of preliminary networks. The final network architecture had 7 inputs, one hidden layer with 10 hidden units, and a single output. The output unit represents the outgoing average air flow rate.

Since the data set was small (only 58 observations), a cross validation method was used to evaluate the performance of the application network. This approach was chosen in favor of a group cross validation approach because it provides a better estimate of the performance of the final network. Fifty eight validation networks were built using the same parameters as the application network with an upper bound of 10 hidden units. This upper bound, which is the same as the number of hidden units for the application network, limits the number of hidden units chosen by the cascade-correlation algorithm for the validation networks. Each validation

network was trained on 57 observations and tested on the hold out observation. Each network had a different hold out observation as its test set. The test set errors obtained from all 58 cross-validated networks provides an estimate of the generalization ability of the application network.

The final network was able to predict the outgoing average air flow rate with a mean absolute error of 0.0972 (0.0569%) and a root mean squared error of 0.1358 (0.0794%). The R-squared (coefficient of determination) value of the final network, which was estimated by the validation networks, is 0.8741 which proves to be somewhat superior to the regression model. Figure 6 provides a visual relationship between the predicted and the actual observed outgoing average air flow rate of the cross validation networks. Although the predictions of the application network were expected to be fairly accurate, the precision level of the model was still not high enough for use in the plant. Additional data has to be gathered and more information on the condition of the media will have to be collected in order to improve the model.

Insert Figure 6 here

Chemical Oxidation Application

The cyclohexane oxidation process is used to produce cyclohexanol and cyclohexanone. These products are then used to generate caprolactam and adipic acid, which are eventually consumed as prime raw materials for the nylon-6 and nylon-6,6 polymerization processes. Conventionally, cyclohexane oxidation is the reaction between liquid cyclohexane and air. The reaction can be controlled in an experimental setting [Tekie et al., 1997] where the following parameters can be adjusted/changed in order to obtain measures of the volumetric mass transfer coefficient ($k_L a$):

- mixing speed of the reactor, which is used to mix the reactants, x_1 ;
- pressure of the feed gas, x_2 ;
- temperature of the reaction environment, x_3 ;
- liquid height of cyclohexane that is above the bottom of the reactor, x_4 ;
- type of feed gas (nitrogen or oxygen);
- type of reactor (gas-inducing reactor, GIR, or surface-aeration reactor, SAR).

A central composite experimental design was carried out to collect data for the oxidation process of liquid cyclohexane. Based on the design of experiments data, the study of the effects of these variables on $k_L a$ values helped to develop a quadratic response surface model [Tekie et al., 1997] given in Equation (1):

$$\ln(k_L a) = b_0 + \sum_{i=1}^4 b_i x_i + \sum_{i=1}^4 b_{ii} x_i^2 + a_1 \exp(g_1 (x_1 + g_2)^2) + a_2 \exp(g_3 (x_1 + 3)(4 - x_4)) \quad (1)$$

However, this model can only be applied to a specific combination of gas type and reactor type. For the experiments carried out by Tekie et al., there were a total of four different combinations of gas and reactor. Therefore, the authors developed four different quadratic response surface models, each with a different set of parameters (i.e., b's, a's, and g's) for each model. This approach, however, cannot be used to generalize to a larger set of gas/reactor combinations without re-estimating the equation parameter set. Furthermore, their approach required a considerable amount of effort to fine tune the functional form and the parameters.

Neural Network Modeling for Chemical Oxidation Process

The use of neural networks is motivated because of their accommodation of non-linearities, interactions, and multiple variables. Moreover, a generalized approach for predicting the volumetric mass transfer coefficient can be achieved while considering the operating

variables (temperature, pressure, mixing speeds and liquid heights) along with gas types and reactor types as input variables. This approach can be eventually used to optimize the oxidation process while considering variations in gas and reactor.

The data set collected by Tekie et al. was used for construction of the networks. After processing and purifying the data, the final set had 296 observations. The training parameters, network architectures and stopping points were identified via preliminary experiments. An ordinary backpropagation algorithm was used. The final application network had six inputs, one hidden layer with eight hidden units and one output. The output unit represents the volumetric mass transfer coefficient, $k_L a$. This network was developed using the entire data set of 296 observations. Similar to the example from ceramic slip casting, a group cross validation method was used to validate the application network. More specifically, a 74 group cross validation approach, which required constructing 74 validation networks, was carried out. First, the entire data set was randomly divided into 74 disjoint groups of data (each group had four observations). Then each validation network was trained using 73 groups of data and tested on the hold back group. Combining all 74 test sets exhausts the original data set.

Table 4 summarizes the error measures and the R-squared values of the application network and the validation networks. The R-squared value of the application network, which was calculated by the test set errors of the validation networks, is 0.9773. Therefore, the application network can explain about 98 percent of the variation of the volumetric mass transfer coefficient.

Insert Table 4 here

Figure 7 describes the relationship between the predicted and the target volumetric mass transfer coefficient for the validation networks. It shows that the application network is expected to provide very accurate predictions.

Insert Figure 7 here

Concluding Remarks

Three diverse neural network predictive process models were presented using real world engineering problems. The ceramic slip casting application was part of a larger project for which only the neural network development was discussed in this chapter. The final product of this project has been implemented at a major U.S. manufacturer of sanitary ware to improve the product quality and the production efficiency [Lam et al., forthcoming]. The second example is a collaboration between a machining company, two automotive companies and the University of Pittsburgh. This project is currently underway and this chapter discussed some of the more recent results in the model building phase of the abrasive flow machining process. The last example demonstrates a more generalized approach to model the chemical oxidation process of cyclohexane. This approach does not require the construction of multiple functional models for each combination of gas and reactor and can be used for multiple reactor and gas combinations.

Defining Terms

Application network: The network that is ultimately used for the manufacturing application.

Cross validation: Also known as leave-one-out cross validation. This approach requires the construction of n validation networks, where each is built using $n-1$ observations and tested on the left-out point. Combining all the test sets exhausts the original n observations.

Data splitting: Requires splitting the available data into two sets: a training set and a testing set, where the training set is used to train the network and the testing set is used to evaluate the performance of the network.

Group cross validation: Also known as leave-k-out cross validation. This approach is similar to cross validation, except that k observations are held back each time.

Validation networks: Defined as the additional networks constructed to infer the performance of the application network.

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Table 1. Slip Casting Process Parameters.

<u>Input</u>	<u>Parameter</u>	<u>Definition</u>
1	Plant Temperature (°F)	The temperature of the plant.
2	Relative Humidity (%)	The humidity level of the plant.
3	Cast Time	The time duration that the liquid slip is left in the mold before draining.
4	Sulfate (SO ₄) Content	The proportion of soluble sulfates in the slip.
5	Brookfield - 10 RPM	Viscosity of the slip at 10 revolutions per minute.
6	Brookfield - 100 RPM	Viscosity of the slip at 100 revolutions per minute.
7	Initial Reading	Initial viscosity (taken at 3 1/2 minutes).
8	Build Up	Change in viscosity from initial reading (taken after 18 minutes).
9	20 minute Gelation	Thixotropy (viscosity versus time).
10	Filtrate Rate	The rate at which the slip filtrates.
11	Slip Cake Weight	Approximation of the cast rate without considering a mold.
12	Cake Weight Water Retention	Moisture content of the cake. See slip cake weight.
13	Slip Temperature	The temperature of the slip.

Source: Lam, S. S. Y., Petri, K. L. and Smith, A. E., "Prediction and Optimization of a Ceramic Casting Process Using A Hierarchical System of Neural Networks and Fuzzy Logic," *IIE Transactions*, to appear.

Table 2. MAE and RMSE for the Moisture Gradient Network.

<u>Network</u>	<u>MAE</u>	<u>RMSE</u>
Application Network	0.0025	0.0045
Validation Networks	0.0036	0.0061

Table 3. MAE and RMSE for the Cast Rate Network.

<u>Network</u>	<u>MAE</u>	<u>RMSE</u>
Application Network	0.0156	0.0207
Validation Networks	0.0167	0.0243

Table 4. MAE, RMSE and R-Squared Values for the Oxidation Network.

<u>Network</u>	<u>MAE</u>	<u>RMSE</u>	<u>R-Squared</u>
Application Network	0.00067	0.00106	0.9856
Validation Networks	0.00079	0.00133	0.9773

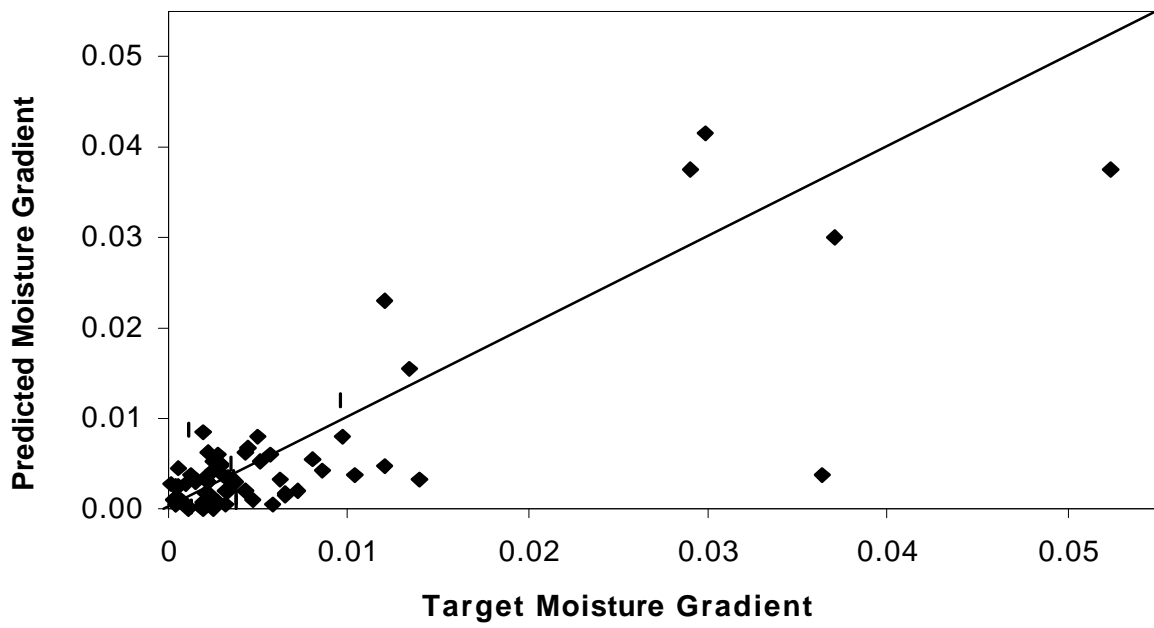


Figure 1. Performance of a Typical Cross Validation Network for Moisture Gradient.

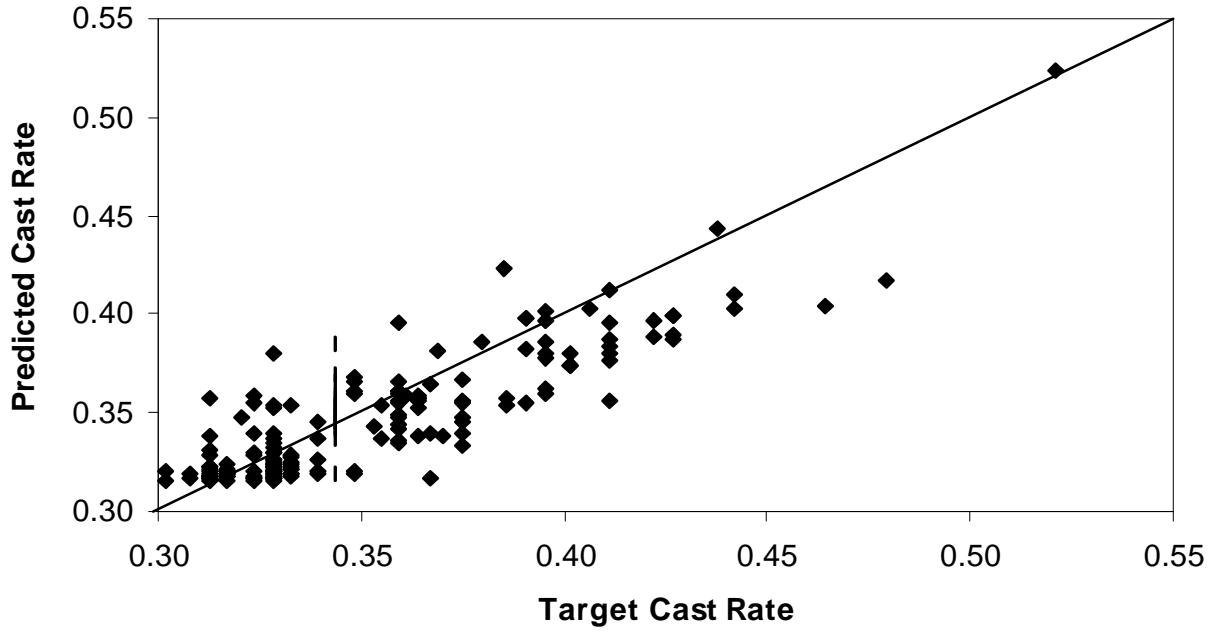


Figure 2. Performance of a Typical Cross Validation Network for Cast Rate.

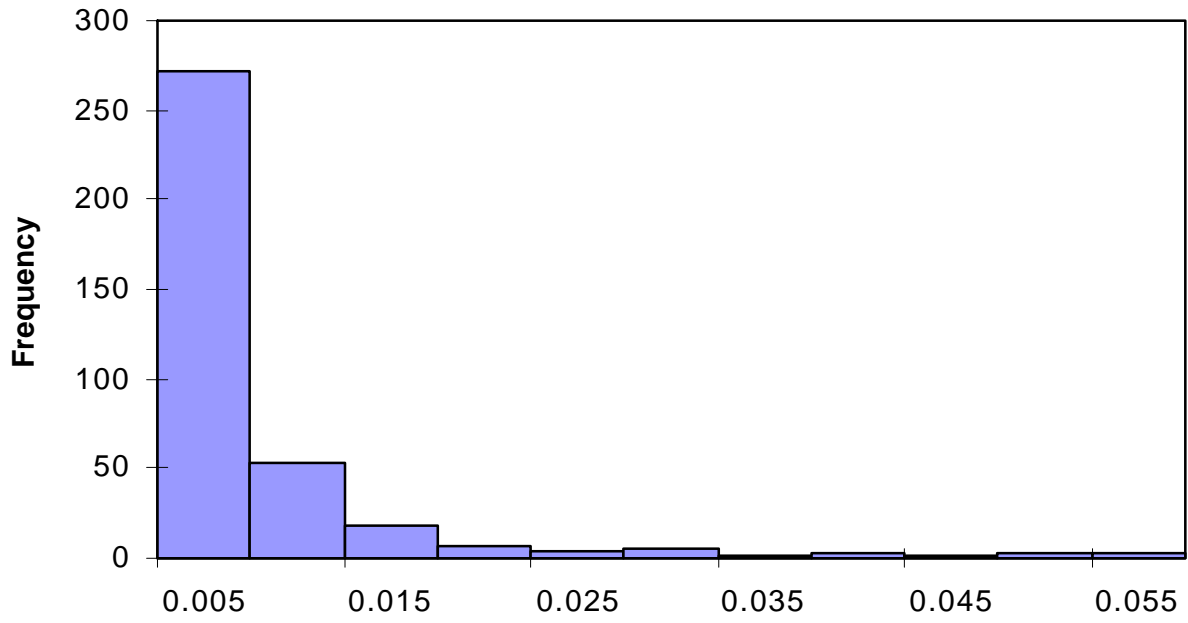


Figure 3. Data Distribution of Moisture Gradient.

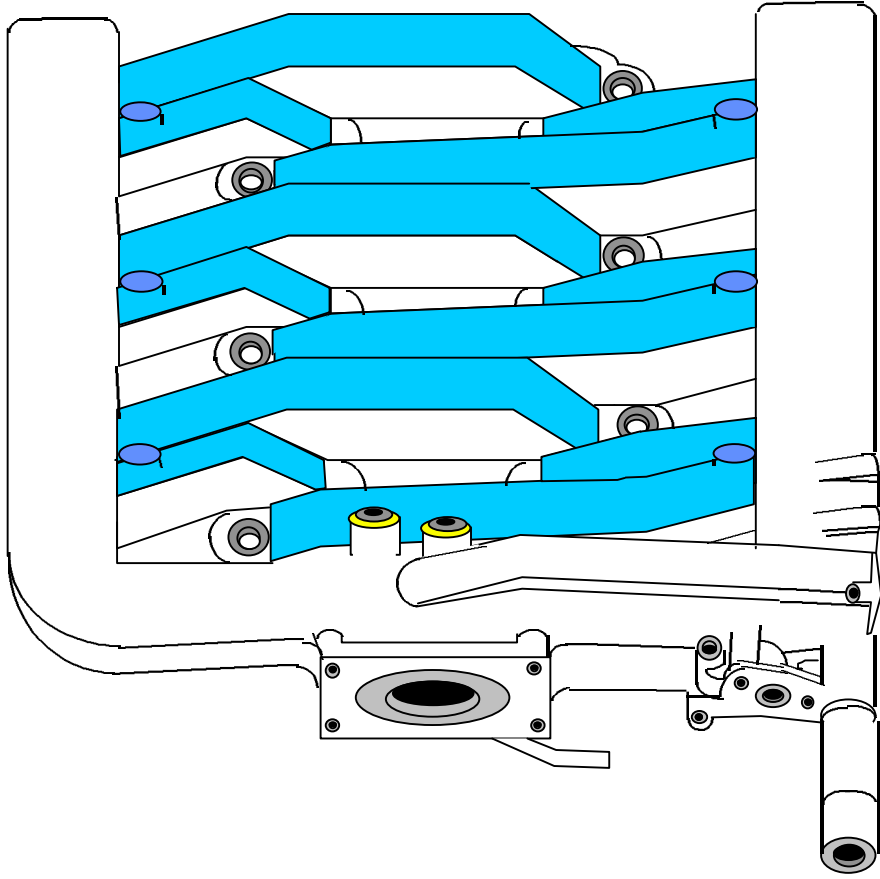


Figure 4. Drawing of an Engine Manifold.

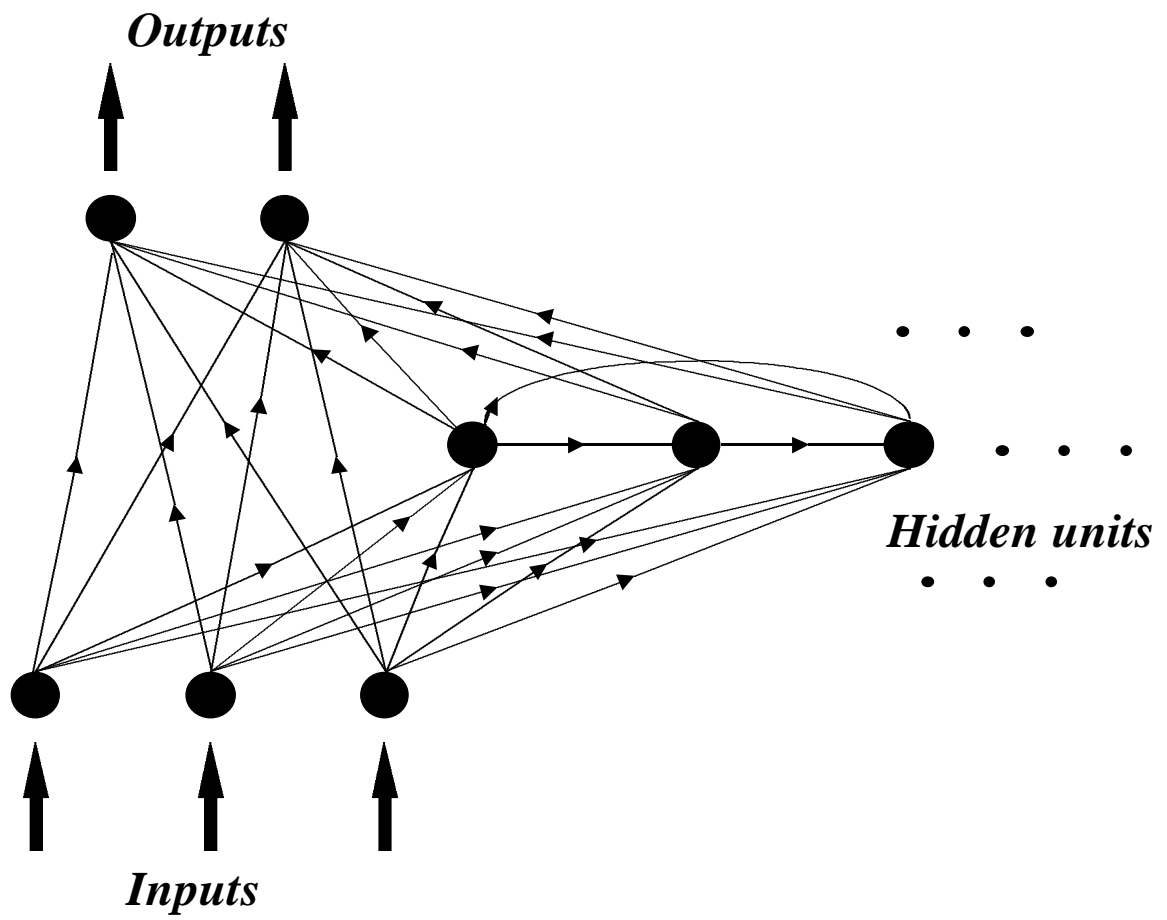


Figure 5. A Typical Cascade-Correlation Neural Network.

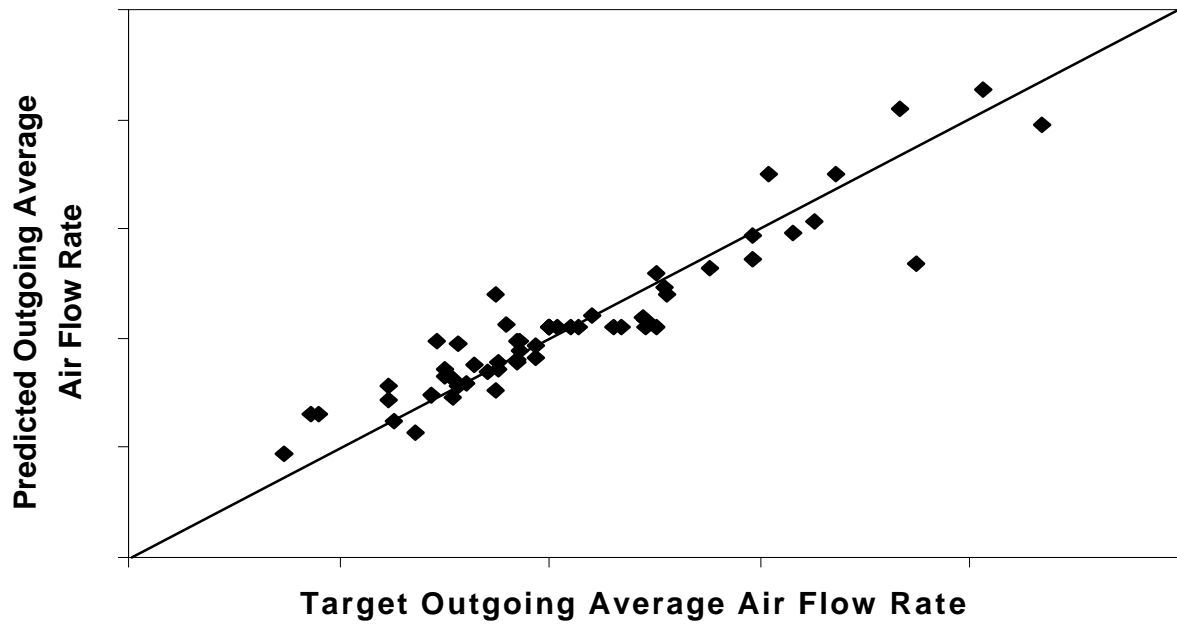


Figure 6. Performance of Cross Validation Networks for the Cascade Application Network.

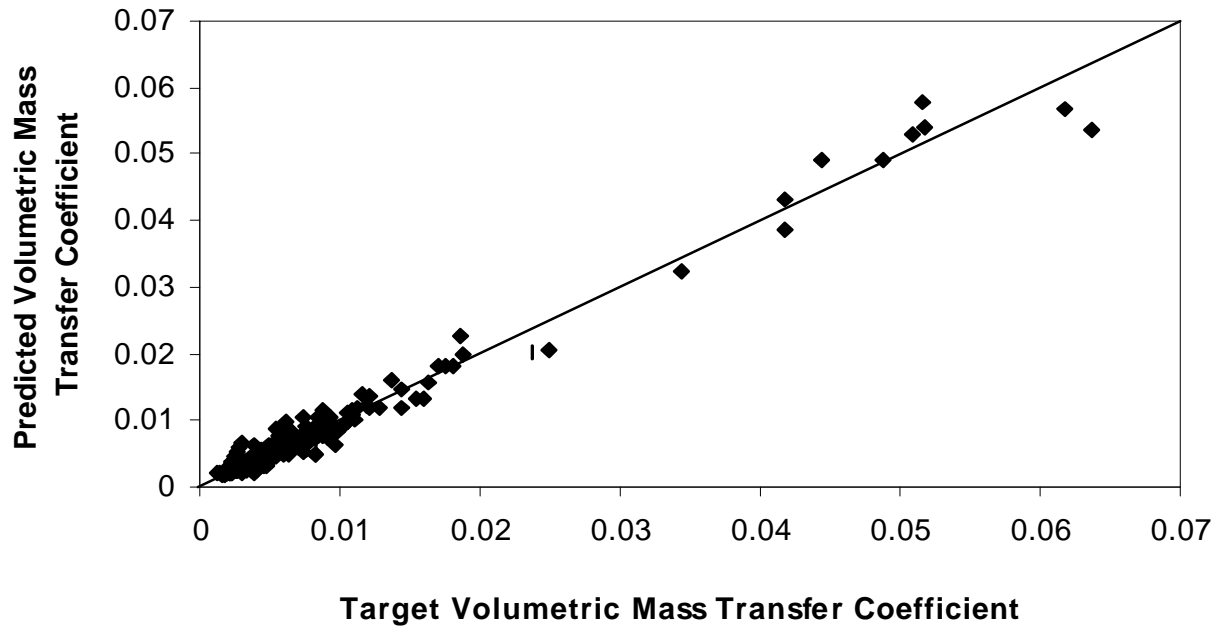


Figure 7. Performance of Validation Networks for the Oxidation Process.