

# MODELLING OF AN INDUSTRIAL FLUID CATALYTIC CRACKING UNIT USING NEURAL NETWORKS

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An artificial neural network (ANN) model for determining the steady-state behaviour of an industrial Fluid Catalytic Cracking (FCC) unit is presented in this paper. Industrial data from a Greek petroleum refinery were used to develop, train and check the model. FCC is one of the most important oil refinery processes. Due to its complexity the modelling of the FCC poses a great challenge. The proposed model is capable of predicting the volume percent of conversion based on six input variables. This work is focused on determining the optimum architecture of the ANN, in order to gain good generalization properties. The results show that the ANN is able to accurately predict the measured data. The prediction errors in both training and validation data sets are almost the same, indicating the capabilities of the model to accurately generalize when presented with unseen data. The neural model developed is also compared to an existing non-linear statistical model. The comparison shows that the neural model is superior to the statistical model.

*Keywords: fluid catalytic cracking; process modelling; neural networks; multi-layer perceptron.*

## 1. INTRODUCTION

Fluid catalytic cracking (FCC) is an important oil refinery process, which converts high molecular weight oils into lighter hydrocarbon products. Industrial FCC units are designed to be capable of using a variety of feedstocks, including straight run distillates, atmospheric and vacuum residua and vacuum gas oils. They produce a range of products, which must adapt to seasonal, environmental and other changing demand patterns. Since FCC units are capable of converting large quantities of heavy feed into valuable lighter products, any improvement in design, operation or control can result in substantial economic benefits.

A typical FCC unit is shown in Figure 1. It consists of two interconnected gas-solid fluidized bed reactors. The riser reactor, where almost all the endothermic cracking reactions and coke deposition on the catalyst occur, and the regenerator reactor, where air is used to burn off the coke accumulated on the catalyst. The heat produced is carried by the catalyst from the regenerator to the reactor. Thus, in addition to reactivating the catalyst, the regenerator provides the heat required by the endothermic cracking reactions. The region of economically attractive operational conditions is determined by both the properties of the feedstocks and catalyst and the desired product distribution requirements<sup>1</sup>. In practice, the optimization of the FCC unit to the desired range of products is usually carried out by trial and error. The disadvantage of this approach is that the transition from one state to the other must be gradual and it is not always successful, because of the complex interactions between the two reactors. As a result, it could lead to loss of production and consequently affect profits<sup>2</sup>.

Process modelling can be used to discover the optimal

path for a safe plant movement of one state to another, which minimizes product loss during the change. A process model is a functional relationship among variables that explains the cause and effect relationships between inputs and outputs. Models can be developed from fundamental principles, such as the laws of conservation of mass, energy and momentum, and other chemical engineering principles. Such models are capable of explaining the underlying physics of the system and are called phenomenological models. Many phenomenological models for the FCC process have appeared in the literature<sup>1-6</sup>. However, due to the complexity of the industrial FCC units, it is very difficult to obtain accurate phenomenological models. The complexity arises from the strong interactions between the operational variables of the reactor and the regenerator. Moreover, there is a large degree of uncertainty in the kinetics of the cracking reactions and catalyst deactivation by coke deposition in the riser reactor and the coke burning process in the regenerator<sup>4</sup>. Even if an accurate phenomenological model is obtained, it may be highly complicated and require simplifying assumptions for its solution<sup>1</sup>.

Another method for practical process modelling is the black box approach, where models are obtained exclusively from experimental plant data. Such models do not provide a detailed knowledge of the underlying physics of the problem, but they do provide a description of the dynamic relationship between input and output variables. Statistical models based on regression analysis is an example of such a black box approach<sup>7</sup>. However, the most common approaches rely on linear system identification models. Unfortunately, the majority of processes found in the chemical industries are non-linear and in these cases the performance of the linear models can be inadequate.

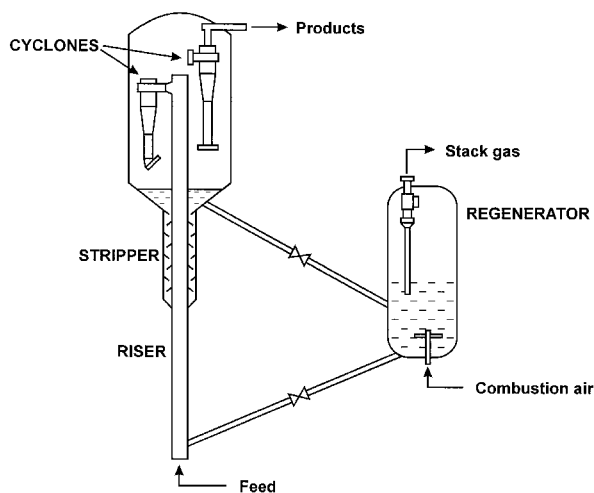


Figure 1. A typical FCC unit.

Recently a promising alternative modelling technique, artificial neural networks (ANNs), has found numerous applications in representing non-linear functional relationships between variables. ANNs are mathematical models, which try to simulate the brain's problem solving approach. Although ANNs are not new in concept, interest in process modelling has increased significantly in the last decade. Some reasons for this growing interest are the tremendous evolution of digital computing, the limitations of traditional modelling techniques, the suitability for non-linear multi-variable systems and the low cost of development<sup>8</sup>. Some important published applications of ANNs in chemical engineering are: fault diagnosis in chemical plants<sup>9–11</sup>, dynamic modelling of chemical processes<sup>12,13</sup>, system identification and control<sup>14,15</sup>, sensor data analysis<sup>16</sup>, chemical composition analysis<sup>17,18</sup>, and inferential control<sup>19</sup>. Joseph *et al.*<sup>20</sup> performed a comparison between classical statistical methods and ANNs. They concluded that ANN models perform better than regression models and show more tolerance to noise in the data.

McGreavy *et al.*<sup>21</sup> reported an extensive study on the use of ANNs to model FCC units. They developed four models to predict the hydraulic parameters of the fluid bed. A separate reaction model was used to predict the product distribution. The predicted parameters are in good agreement with the measured data. However, the averaged predicted error in product distribution increased by a factor between 3 and 21, when the model was used to predict new unseen data. This behaviour clearly shows the importance of a proper ANN selection procedure, which guarantees the high generalization abilities of the model.

In this paper a feed-forward ANN model is developed and trained on measured data from an industrial FCC unit. The model is capable of predicting the volume percent of conversion under steady-state conditions, based on six input variables. Special attention is given to the steps required to achieve an optimal performing model with good generalization properties. This model can be a useful tool for catalysts and feedstocks evaluation, optimization of the operating conditions and also during the design phase of FCC units. The structure of the paper is as follows: a description of the modelling approach followed in this study is given in section 2. Section 3 provides a description of the

data set used for developing the model. Then, in section 4, the step-by-step procedure for the selection of the optimal ANN structure is presented. Section 5 presents the simulated results obtained by the optimal ANN model and provides a comparison with a regression model. Concluding remarks are presented in section 6.

## 2. THE NEURAL NETWORK APPROACH

ANNs basic premise is that the interactions among a large number of simple computing elements, called nodes or neurons, can effect complex information processing. There exist many network architectures<sup>22</sup>. In this work, a fully connected, feed-forward network, widely known as multi-layer perceptron (MLP), is considered (Figure 2). This type of network is especially suited to modelling highly non-linear relationships and to accurately generalizing when presented with unseen data<sup>7</sup>. The nodes are arranged to form an input layer, one or more hidden layers and an output layer, with nodes in each layer connected to all nodes in neighbouring layers. Typically one hidden layer has been found to be sufficient in most applications<sup>7</sup>. A real valued number called 'connection weight' or simply 'weight' is associated with each connection. The role of the weights is to modify the signal carried from one node to the other and either enhance or diminish the influence of the specific connection.

Nodes in the input layer are not associated with any calculations. They act as distribution nodes and transfer the inputs to the nodes of the first hidden layer. The outputs from the output layer represent the network's predicted outputs. The function of any node in the hidden and output layer is to receive a number of inputs from the previous layer, sum the weighted inputs plus the bias, non-linearly transform the sum via an activation function and finally broadcast the output either to nodes of the next layer or to the environment. Referring to Figure 2, the output,  $z_l$ , of the  $l^{\text{th}}$  hidden node is given by:

$$S_l = \sum_k (w_{kl}x_k - \theta_l) \quad (1)$$

$$z_l = f(S_l) = \frac{1}{1 + \exp(S_l)} \quad (2)$$

where  $w_{kl}$  is the weight for the connection from the  $k^{\text{th}}$  input node to the  $l^{\text{th}}$  hidden node and  $\theta_l$  is the bias. In this case a

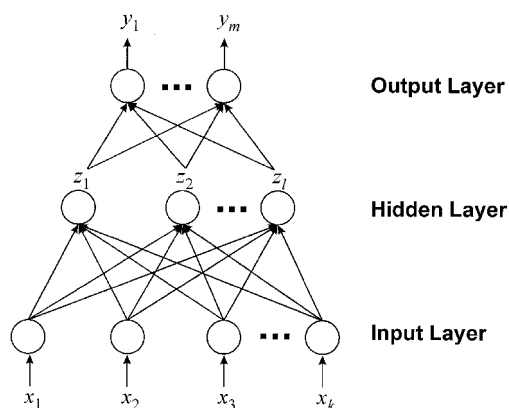


Figure 2. The basic architecture of a feed-forward neural network with a single hidden layer.

logistic sigmoid relationship has been used as activation function.

The steps involved in every effort to build a functioning ANN model of an industrial process are:

- **Data collection.** For effective modelling the data must be information rich over a wide operating range. Since in chemical plants time to steady state can take several hours, plant tests must be conducted over several days continuously.
- **Data preprocessing.** Raw data obtained from plant tests cannot be used in identification studies. They have to be filtered to remove unmeasured noise and outliers that may have been caused by some measurement error.
- **Model selection.** The structure of the network needs to be specified. The specification includes the number of hidden layers and the number of nodes in each hidden layer. The number of nodes in the input and output layers are determined by the plant inputs and outputs.
- **Training and validation.** During supervised training, the network learns by adapting its weights based on the training data set provided at the input and output layers. The ANNs used in this study were trained using the EBP (Error-Back-Propagation) algorithm, which is implemented in the Stuttgart Neural Network Simulator. This simulator allows neural networks to be easily designed and trained and is freely available via the Internet (<http://www.informatik.uni-stuttgart.de/ipvr/bv/projekte/snns/snns.html>). The weights are determined by iteration to produce the minimum error in the output, measured, for example, as the root mean squared error:

$$RMS = \sqrt{\frac{\sum_p \sum_m (y_m^p - d_m^p)^2}{p m}} \quad (3)$$

where  $p$  represents the examples in the training set,  $d_m^p$  is the desired output of  $m^{\text{th}}$  node on  $p^{\text{th}}$  example and  $y_m^p$  is the predicted output. Parameters such as learning rate and momentum used in the EBP and other mathematical details about the EBP algorithm are discussed elsewhere<sup>23</sup>. For the purpose of model building, the available data are split into two different sets: training set and validation set. The ANN is trained using the training data set. To avoid overtraining<sup>8</sup>, the network performance with respect to data of the validation set is monitored after each training iteration. Thus, the validation set is used to gauge the generalization performance of the model. The training is stopped at the point where the *RMS* of the validation set starts to increase. Because the performance of the EBP algorithm depends on the initial values of weights, several runs with different initial random weights need to be performed.

In order to achieve an optimal performing network, the steps of model selection, training and validation need to be iterated. A different network structure (number of hidden layers and/or number of hidden nodes) is examined in each iteration. The network with the minimum validation error is considered to be the optimum for the process examined. Details on this procedure are given in section 4.

### 3. THE DATA SET

The training and validation of the ANN model was based upon industrial data provided by the Aspropyrgos Refinery of Hellenic Petroleum S.A. (Athens). The data sets were

Table 1. ANN model variables and their ranges.

Variable	Range
Conversion: $Y$ (vol %)	70.74 to 85.18
Specific gravity of feed: $SG$	0.90 to 0.92
Sulphur content of the feed: $S$ (wt %)	0.22 to 2.08
Catalyst to oil ratio: $C/O$	4.48 to 6.33
Specific area of the catalyst: $SA$ ( $\text{m}^2 \text{g}^{-1}$ )	114 to 154
Catalyst circulation rate: $CCR$ ( $\text{tn min}^{-1}$ )	14.18 to 20.36
Temperature at the exit of the riser: $T$ ( $^{\circ}\text{C}$ )	514.7 to 518.7

collected once a week for a period of two years. Excluding the months where a unit shut-down occurred, a total of 92 observations were provided. In selecting data for model building, however, it is important to ensure that it represents normal operating states to avoid spurious predictions from unusual conditions. So, blocks of data corresponding to process faults were excluded from the study. Also, outliers that may have been caused by some measurement errors were removed. A simple outlier detecting method was followed, where any observation that differs more than two standard deviations from the mean is removed from the set. As a result, a set of 50 observations, representative of various operating conditions and a broad range of the input variables, was used for the development of the ANN model. The output of the model consists of the volume percent of conversion ( $Y$ ). The input variables include properties of the feedstock, properties of the catalyst and operating conditions. The variables of the model and their ranges are summarized in Table 1. The training of the ANNs was carried out on a subset of 40 random observations that included the minimum and maximum values of each variable. The remaining 10 observations were used for validation purposes.

In order to be used with the ANNs models, all the data were normalized into the range 0 to 1. This was carried out by determining the maximum and minimum values of each variable and using the following formula:

$$x_{\text{norm}} = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} \quad (4)$$

A similar formula was used to return the predicted normalized conversion to its original units.

### 4. DEVELOPMENT OF THE NEURAL MODEL

In this section the procedure for selecting the optimal performing ANN model for the FCC unit is presented. The task is to find the network structure, which gives the minimum error in the validation data set. Only the case of one hidden layer is studied. The number of nodes in the input and output layers is 6 and 1 respectively, equal to the number of input and output variables. Therefore, the goal is to find the optimum number of nodes in the hidden layer. There are several methods about the determination of the optimum number of hidden nodes. These methods are based either on heuristic network derivation such as 'regularization', 'pruning' and 'stopped training', or statistical principles such as 'hypothesis testing', 'information criteria' and 'cross validation'. Although the determination of the optimum number of hidden nodes is still under intensive study, it seems that statistical methods have more benefits

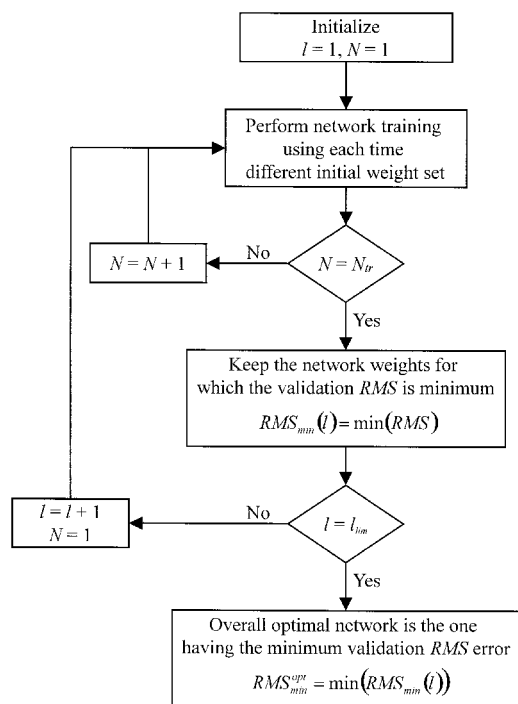


Figure 3. Flowchart showing the steps involved in creating an optimally performing ANN model.

than the heuristic methods<sup>24</sup>. In this work, a trial and error procedure based on cross validation was followed. This method is presented in Figure 3.

First the number of nodes in the hidden layer ( $l$ ) is set at its minimum value ( $l = 1$ ). Then the network is trained as explained in section 2. The training procedure is repeated several ( $N_{tr}$ ) times with a different set of initial weights each time. The network with the minimum  $RMS$  for the validation data set  $RMS_{min}$  is optimal for the particular value of  $l$  and the weight set corresponding to this run is saved. Thereafter,  $l$  is incremented and an optimal network (that is an optimal weight set) for the new value of  $l$  is obtained. The procedure is iterated until  $l$  reaches the value of  $l_{lim}$  that is the upper limit for the number of hidden units. Generally,  $l_{lim}$  depends on the size and the complexity of the problem. In this work it was set to 10. The optimum number of hidden nodes corresponds to that value of  $l$ , for which the

network attains the least  $RMS_{min}$ . It must be noted that, since only a finite number of training runs can be performed to explore the error surface, the optimal weight set obtained may represent a deep local minimum of the error surface and not its global minimum.

The results of this trial and error method are presented in Figure 4. Networks with four and five nodes present similar  $RMS$  errors for the validation data set. However, the network with five nodes gives much better results for the training set and it is considered to be the best for modelling the FCC unit. The results of this neural model are presented in the next section.

## 5. RESULTS AND DISCUSSION

In this section the results of the optimum neural model, which was obtained from the procedure presented earlier in this paper, are discussed and compared to the results of a non-linear statistical model.

### 5.1. Results of the ANN Model

In Figure 5 the measured and the predicted values of the conversion in the FCC unit have been plotted. Training and validation data are all presented on the same plot. The observations from 1 to 40 correspond to the training data set, while those from 41 to 50 are the validation data set. It can be readily seen that the ANN model performs very well in predicting both data sets, not only producing trajectories of the same trend as the process measurements, but being also very close to the majority of the experimental data points. This is more obvious in Figure 6, which represents the scatterplot of measured values of conversion against predictions. In the same figure the best-fit line is also drawn (dotted line). Model predictions that exactly match the measured values would fall on the line with an intercept ( $a$ ) of 0 and a slope ( $b$ ) of 1. Almost all points are very close to this line, where theoretically they should lie.

Table 2 summarizes the main statistical parameters of the ANN model, that is, the root mean square error ( $RMS$ ), the coefficient of determination ( $R^2$ ) and the values of the intercept ( $a$ ) and slope ( $b$ ) as defined above. The last two parameters are universal model comparison statistics that are used to quantify useful information on the systematic error of the model<sup>25</sup>. These statistics are presented for the

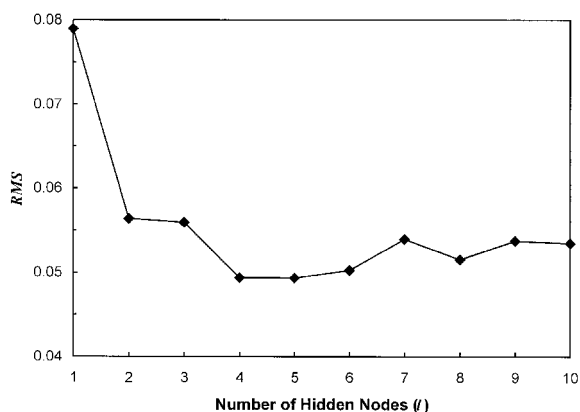


Figure 4. Plot showing the dependence of the minimum RMS error for the validation data set on the number of hidden nodes.

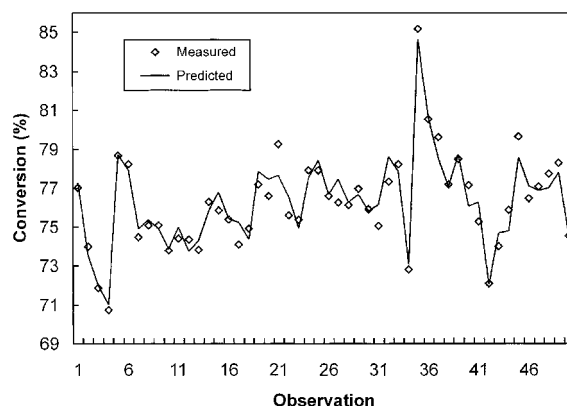


Figure 5. Comparison of measured and predicted values of conversion using the ANN model.

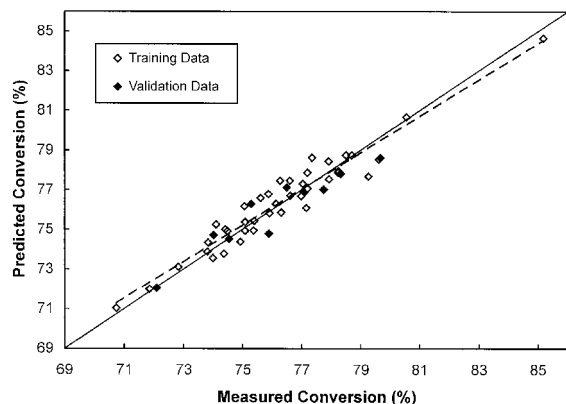


Figure 6. Scatterplot of measured against predicted values of conversion using the ANN model.

training, validation and total data set. The predictions for the training data are better than those for the validation data. This is expected, since the training data are responsible for the definition of the weights of the neural model according to the EBP algorithm. Thus, the neural model learns the characteristics of the training data better than any other data. The fact that the values of these parameters for the validation data are similar respectively, proves that the neural model can generalize sufficiently well the knowledge it received from the training data. The ratio of the *RMS* error between validation and training data sets is only 1.09, which can be considered as a significant improvement over previous efforts to model FCC process<sup>21</sup>.

## 5.2. Comparisons with a Statistical Model

The excellence of the neural model is better shown, when it is compared to a statistical model developed by Theoharopoulos<sup>26</sup>. This model is based on a generalized equation proposed by Wollaston *et al.*<sup>27</sup> and has the following form:

$$\frac{Y}{100 - Y} = \frac{(C/O)^A \cdot CCR^F \cdot SA^G \cdot \exp(H/RT)}{(SG + B)^1 \cdot (S + C)^D} \quad (5)$$

where  $R = 1.9872 \text{ cal mol}^{-1} \text{ }^\circ\text{C}^{-1}$  and  $A, B, C, D, F, G, H$  and  $I$  are adjustable parameters. The independent variables of the above model are the same as those used in the ANN model and are described in Table 1. The parameters of this model can be easily determined with the method of non-linear regression analysis. In this work, the following values were obtained based on the same data set used to train the ANN model:  $A = 0.6650$ ,  $B = 0.1048$ ,  $C = -0.1985$ ,  $D = -0.0571$ ,  $F = -1.2513$ ,  $G = 0.8403$ ,  $H = 20.6070$ ,  $I = 26.7789$ .

The regression model's predictions are not that accurate compared to those of the ANN model. Schematically, this is

Table 2. ANN model statistics for the training, validation and total data set.

	Training data	Validation data	Total
<i>RMS</i>	0.65	0.71	0.67
$R^2$	0.93	0.89	0.92
$a$	6.18	13.13	7.15
$b$	0.92	0.83	0.91

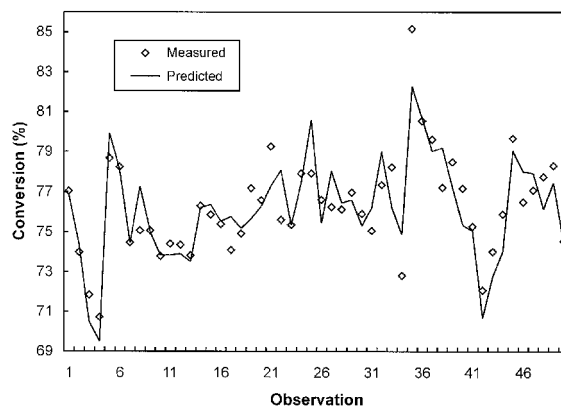


Figure 7. Comparison of measured and predicted values of conversion using the non-linear statistical model.

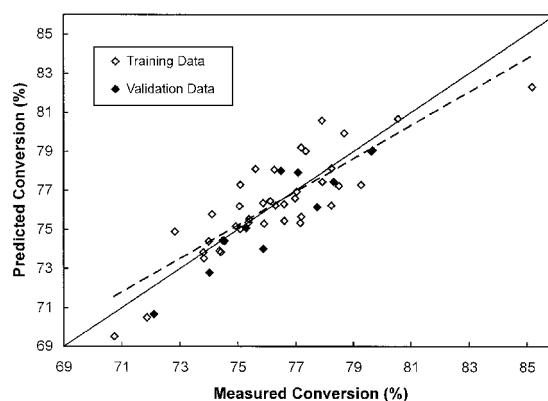


Figure 8. Scatterplot of measured against predicted values of conversion using the non-linear statistical model.

shown by the predicted line in Figure 7, which fails to depict more trends in both the training and validation set than the ANN model in Figure 5 respectively. This is clearer in Figure 8, where the predictions of the regression model are much more scattered than those in Figure 6. In the same Figure the best-fit line is drawn and the results for parameters  $a$  and  $b$  are shown in Table 3. Both parameters  $a$  and  $b$  differ more, compared to those of the neural model, from the ideal values of 0 and 1 respectively. Table 3 also summarizes the main statistical parameters of the regression model. All the parameters, compared to those of the ANN model in Table 2, show the inferiority of the predictions of the regression model.

In Figure 9 the errors of the two models are compared for every observation in the training and validation data set. Although there are single cases, where the error of the

Table 3. Regression model statistics for the training, validation and total data set.

	Training data	Validation data	Total
<i>RMS</i>	1.31	1.17	1.28
$R^2$	0.72	0.69	0.71
$a$	10.95	-6.90	7.96
$b$	0.86	1.08	0.89

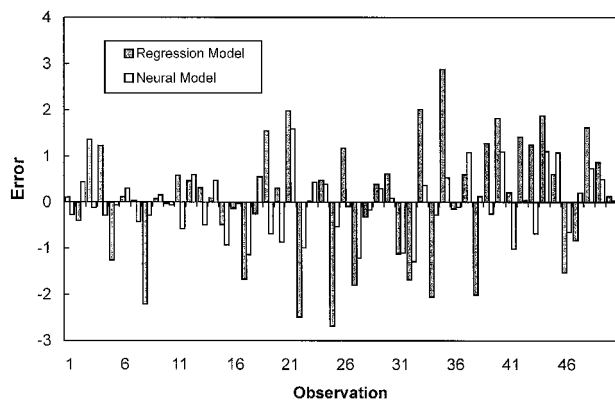


Figure 9. Comparison of prediction errors between ANN and statistical model.

regression model is lower, the superiority of the neural model in general is again obvious.

Although the neural model predicts better than the statistical model, the neural model has about 5 times more adjustable parameters (41) than the statistical model (8). But this is not the main reason why the neural model has better performance. It is not accurate to say that parameter addition will improve the performance of the statistical model because it may lead to overfitting.

## 6. CONCLUSIONS

In this paper, a feed forward neural network model for a fluid catalytic cracking (FCC) unit was developed. The model is trained on measured data from an industrial FCC riser reactor. Special attention was paid to achieving an optimal performing model with good generalization properties. The results indicate that accurate predictions can be made even with a limited training data set. The difference in predictions on training and validation data is minor, reflecting the abilities of the model to accurately generalize when presented with unseen data. Comparisons between the ANN model and a non-linear statistical model clearly show the superiority of the ANN in terms of prediction accuracy. Concluding, the highly non-linear behaviour of the FCC process can be modelled successfully by utilizing the techniques of artificial neural networks.

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