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ANALYSIS AND OPTIMIZATION OF GAS-CENTRIFUGAL SEPARATION OF URANIUM ISOTOPES BY NEURAL NETWORKS

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ABSTRACT

Neural Networks are an attractive alternative for modeling complex problems that show too many difficulties to be solved by phenomenological model. A feed-forward neural network was used to model a gas-centrifugal separation of uranium isotopes. The prediction showed good agreement with the experimental data. An optimization study was performed. The optimal operation condition was tested by a new experiment and a difference of less than 1% was found.

I. INTRODUCTION

The prediction of the separation of uranium isotopes by gas centrifuge process employing mathematical models is quite difficult. The calculations require the simultaneous solution of the equations of gas motion (equation of continuity, the Navier-Stokes equation and equation of energy) and the diffusion equation. The diffusion equation may be solved independently of the equations of gas motion, since the mass difference between uranium isotopes is fas smaller than the avarage of the masses, after the equations of gas motion are solved.

The separation analysis of the countercurrent centrifuge was first defined by Cohen [1] in the 40's through solution of the diffusion equation by using the method developed by Furry, Jones & Onsager [2] for the thermal diffusion column. This became a classical solution, named the Cohen-Onsager equation. This solution made many simplifications, like a constant axial countercurrent flow and a radial averaged concentration. These simplifying hypotheses, which introduce errors when comparing the results with actual centrifuges, have gradually been improved (Olander [3]). Recent works have resorted two-dimensional analytical or numerical analysis (Soubbaramayer [4], Makihara & Ito [5]). Kai [6] reviewed the studies performed by Power Reactor and Nuclear Fuel Development Corp. (PNC), developing a two-dimentional numerical model, considering the non-linear system, but also emphasizing the difficulties of predicting the separative performance of a gas real centrifuge.

The solution of these model-based equations, analytically or numerically, always requires the use of approximations, by linearization of the equations. Consequently, none of the existing methods of calculation are valid for an actual centrifuge, although they are valuable for understanding the physical phenomena that take place in the gas centrifuge.

We propose here the use of neural networks for the simulation and prediction of the separative performance of a gas centrifuge. A neural network, due to its parallel characteristics, is able to "learn" the non-linearity of a process presented to the network in the training set.

II. NEURAL NETWORK

Neural networks are one of the fastest growing areas of artificial intelligence, particularly in Chemical and Nuclear Engineering. The main applications are in fault diagnosis (Hoskins et.al. [7]) and in process control and modeling (Bhat & McAvoy [8], Su & McAvoy [9], Chan & Nascimento [10]). In nuclear technology, the use of neural networks began at the end of the 80's. They have been widely used in High Energy Physics (Denby [11], Peterson [12]) and in Nuclear Power Plants (Uhrig [13], Eryurek et.al.[14]).

The application of neural networks in the simulation of chemical and nuclear processes, specifically in the isotope separation by the gas centrifuge, has great interest due to the non-linearity of the process. This technique leads to numerical models, valid for actual centrifuges, avoiding the difficulties of the phenomenological model described above. The success of this kind of modeling depends strongly on the knowledge of the main variables affecting the process and the availability of a good data base with the necessary information over the desired domain.

There are two main structures for neural networks: (i) the multilayer feedforward network, shown in Figure 1, used for modeling steady state systems, and (ii) the recurrent network, which is better for dynamic modeling.

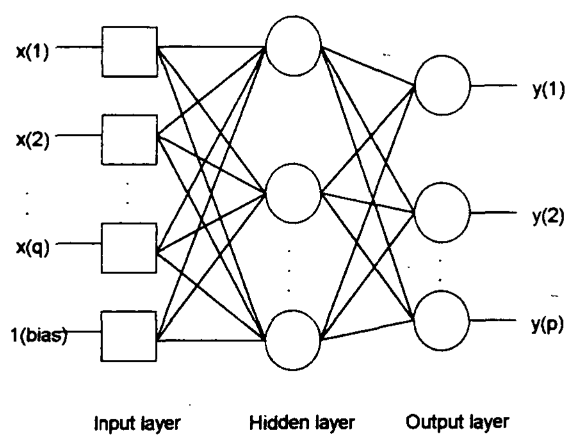

Figure 1. Three Layer Feedforward Neural Network

A neural network is constituted of processing neurons, represented by circles in Fig. 1, and by flow channels that transfer the information between the neurons, named interconnects. The boxes represent neurons where the inputs for the network are stored. Each neuron calculates first the weighted sum of the input signals of the previous layer, and then generates an output through an activation function, usually defined by Eq. (2).

$$S_v = \sum_{u=1}^{n} W_{u,v} x_u + W_{n+1,v} \tag{1}$$

$$f(S_v) = \frac{1}{1+e^{-S_v}} \tag{2}$$

In process modeling, the neural network most used is the three layered network, consisting of an input layer, a hidden layer and an output layer. The input layer consist of $ni+1$ neurons, where ni is the number of input variables, and there is no processing in this layer. Besides the inputs, a bias is given to the network. The inputs are normalized between zero and one in order to help the convergence process. The number of neurons in the hidden layer is defined by the user. According to Pollard [15] the final precision is only slightly sensitive to the number of neurons in the hidden layer after a minimum value. The output layer consists of a number of neurons equivalent to the number of outputs of the process.

The system "learns" by changing the weights ($W_{u,v}$) in such a way as to minimize the sum of the squared differences (E) values expressed by

$$E = \sum_{m=1}^{r} \sum_{k=1}^{p} (y_k^{(m)} - O_k^{(m)})^2 \tag{3}$$

where y_k is the value presented to the neural network in the training set and O_k is the corresponding value obtained in the output layer, calculated by

$$O_k = f(S_k) \tag{4}$$

The backpropagation algorithm is the most used procedure for training three-layered feedforward neural networks (Rumelhart & McClelland [16]). This algorithm is a generalization of the steepest decent method.

III. SIMULATION OF A GAS CENTRIFUGE VIA NEURAL NETWORK

The gas centrifuge, shown in Fig. 2, is basically constituted by a vertical cylinder, of thin wall, rotating at high velocities around its axis, inside a vacuum chamber. The binary gaseous mixture of $^{235}UF_6$ and $^{238}UF_6$ is introduced in this cylinder, named rotor, were it is subjected to the centrifugal forces. That way a pressure distribution is established in the rotor, as a pressure gradient increasing from the axis to the wall. This pressure gradient is different for each isotope, since it is a function of the molecules mass. It results in a partial separation of the isotopes in the radial direction. This partial separation may be multiplied by a countercurrent axial flow, represented in Fig. 2 by the vertical arrows. The countercurrent is induced by internal or external devices. The internal countercurrent flow is induced by thermal drives, like the difference between the temperatures of the end caps or the temperature gradient along the rotor wall, and/or by mechanical drives, like the existence of stationary devices inside the rotor and by the introduction and extraction of material in the rotor.

The separation parameters of a gas centrifuge can be experimentally determined in a separation experiment, for a fixed arrangement of the internal devices of the centrifuge. The centrifuge used was a three-pole centrifuge with the internal fluid flow driven by a stationary scoop at one end of the rotor and a rotating baffle in the other end. In the separation experiment, the pressure of the feed, product and waste line and the mass flows of product and waste are measured. The experiment is run operating the centrifuge in different conditions defined by the flow rates and the output pressure, assuming approximately equal flows of product and waste, in order to study the symmetric case of separation, defined by $\beta=\gamma$. For each operational condition, samples are taken and analyzed to obtain the abundance ratio of each stream processed by the gas centrifuge. A set of 58 experimental results is obtained, each of them consisting in the values of the product and waste flow rates, the pressures in the feed line and in the product and waste throughput, and the abundance ratios of the enriched and depleted material.

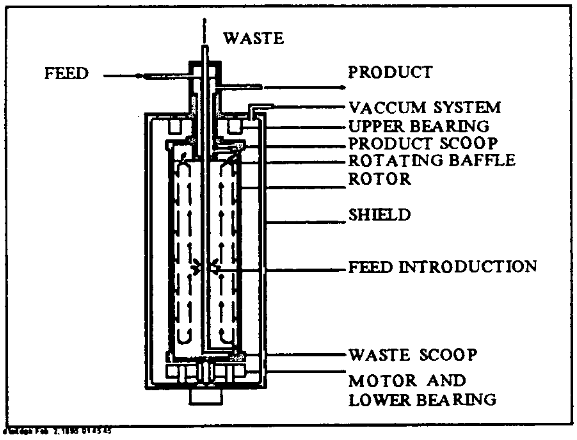

Figure 2. Sketch of a Three-Pole Countercurrent Gas Centrifuge [4]

The application of a neural network approach for the centrifuge was then made, with the following input variables:

- Q_P:mass flow of the product;
- Q_W:mass flow of the waste;
- p_P:pressure in the product line.

and output variables:

- p_F:pressure in the feed line;
- p_W:pressure in the waste line;
- R_P:abundance ratio of the product;
- R_W:abundance ratio of the waste.

The abundance ratio of the feed gas is that of the natural occuring uranium.

Learning And Testing With The Neural Network. The experimental data were divided into two groups: a 'learning set", with 29 data sets, used for the training process of the neural network, and a "test set", with 27 data set, used for checking the training. Each data set results from the mean value of three experimental determinations. A three-layered feedforward neural network was used and trained with the backpropagation algorithm. Four different networks were tested: with 5, 6, 7 and 8 neurons in the hidden layer. The number of presentations employed to train the neural network were 50,000 to 100,000. Table 1 shows the errors calculated in each case for the learning set and for the test set.

TABLE 1. Total Errors Calculated After The Training of Neural Networks With Different Numbers of Neurons in the Hidden Layer

	"LEARNING SET"		"TEST SET"	
NH	N. SETS	RMST	N. SETS	RMSTT
5	100 000	0.123	11 000	0.338
6	100 000	0.070	100 000	0.185
7	100 000	0.056	100 000	0.144
8	50 000	0.114	100 000	0.313

Allowing a larger number of presentations, it was verified that a 100,000 presentations were enough for determining the configuration of the network. The convergence in this case has shown an asymptotic behavior. With these results, a neural network with seven neurons in the hidden layer was chosen. The sum of errors as a function of the number of presentations is shown in Fig. 3 for a network with seven neurons in the hidden layer. In the present case a constant dumping factor was used, since it was not necessary to use a dynamic dumping factor to improve the convergence (Nascimento [17]).

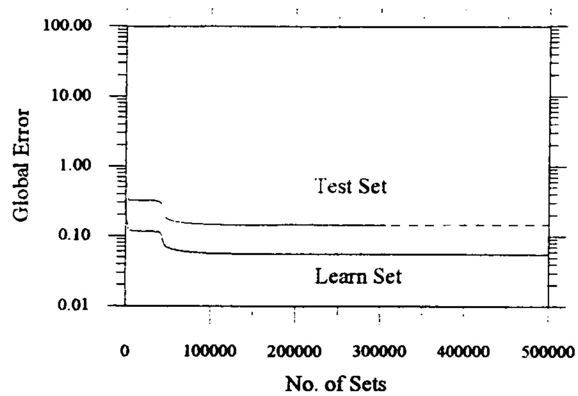

Figure 3. Global Error in the Training of a Neural Network With Seven Neurons in The Hidden Layer:
(a) Learning Set; (b) Test Set

Comparison Of Experimental Versus Calculated Data. After the training of the neural network the weights are chosen so as to minimize the error in the test set. With this network outputs variables are calculated. The primary variables used were the pressures p_F and p_W. However the most important variables in practice are the separation factor α and the separation power δU. The separation power δU represents the separation performance of the centrifuge. The definition of δU is the work required to separate a certain flow of material into two flows of different concentration.

$$\alpha = \frac{R_P}{R_W} \tag{5}$$

$$\delta U = Q_P \frac{R_P - 1}{R_P + 1} \ln(R_P) + Q_W \frac{R_W - 1}{R_W + 1} \ln(R_W) - (Q_P + Q_W) \frac{R_F - 1}{R_F + 1} \ln(R_F) \tag{6}$$

Fig. 4 shows a scheme of the model proposed to calculate the separation parameters of the gas centrifuge using the trained neural network.

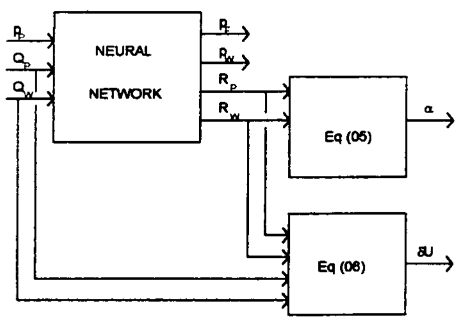

Figure 4. Model for the Calculation of the Parameters of the Gas Centrifuge Using a Neural Network

The comparisons of the primary calculated variables p_F and p_W against the experimental values are shown in Fig. 5 and Fig. 6, respectively. The dashed lines indicate the estimated experimental error. The agreement between the experimental and calculated values for those variables is satisfactory. Normally the training set are always fitted (neural networks as used in this work are called as an universal approximators (Hornik [18])). The most important, however, is the prediction that the neural network showed with the test-set.

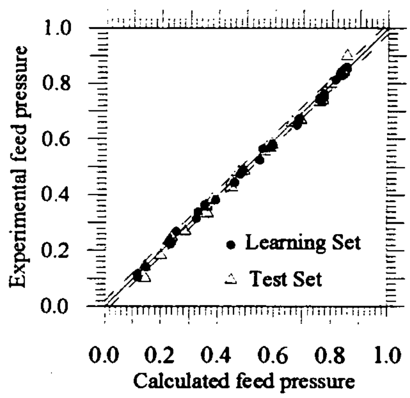

Figure 5. Comparison of the Experimental and the Neural Network Calculated Values of the Pressure in the Feed Line p_f (arbitrary units).

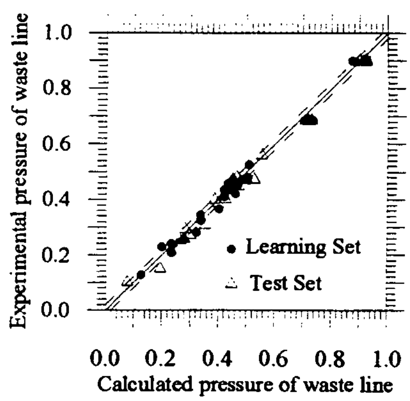

Figure 6. Comparison of the Experimental and the Neural Network Calculated Values of the Pressure in the Waste Line p_w (arbitrary units).

The calculations of the parameters α and δU are performed according to the scheme shown in Fig. 4. The values of the abundance ratios are given by the neural network and the values of α and δU are calculated with Eqs.(5) and (6). Fig. 7 and Fig.8 show the comparisons of the experimental and calculated values of these variables. The reason for calculating the values of α and δU by Eqs. (5) and (6) and not directly from the neural network was because they do not represent primary variables. Normally the values of α and δU are used for design purposes. The comparison of the calculated with the "experimental values" of these variables is in good agreement for both the learning and test sets. A good fitting in the test set means that the neural network can represent well the response surface of the real problem.

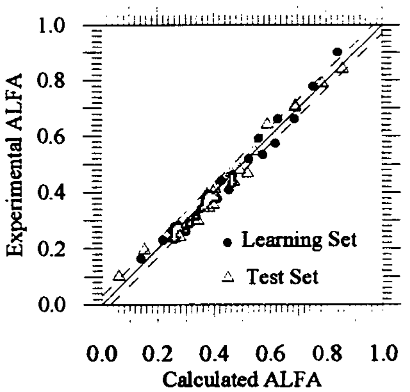

Figure 7. Comparison of the Experimental and the Neural Network Calculated Values of the Separation Factor α

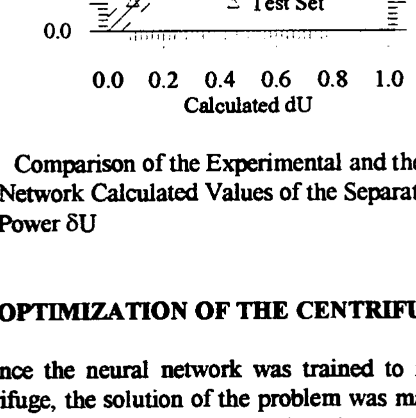

Figure 8. Comparison of the Experimental and the Neural Network Calculated Values of the Separative Power δU

IV. OPTIMIZATION OF THE CENTRIFUGE

Once the neural network was trained to represent the centrifuge, the solution of the problem was mapped on a very fine grid in the domain of the learning set data. Fig. 9 presents a typical surface of the solution of the separative power as a function of the flows Q_P=Q_W and the pressure p_P. With these results, the conditions in which the separative power is maximized can be found by inspection of the surface given by Fig. 9.

A new experiment was then performed under the conditions of the optimized δU, predicted by the simulated surface of δU as a function of Q_P and p_P. The difference between the experimental results and the values calculated using the neural network model was close to 1%.

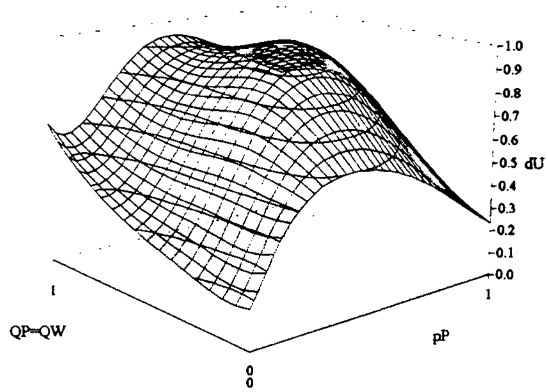

Figure 9. Response Surface for the Separative Power of the Centrifuge

V. CONCLUSION

Modeling by neural networks has been shown an important tool to simulate the separation of uranium isotopes. Experimental data of good quality is fundamental for obtaining reasonable results. The neural network model obtained is valid only for the centrifuge used in the separation experiment. In the present case, the experimental data covered a large domain of variables employed in the model. This fact is very important in order to be confident that the neural network has learned most of the non-linear information of the process. The optimization of the separation of the uranium isotopes was done by inspection of the surface response generated by the neural network. The optimal condition was checked experimentally and the difference of the experimental value was less than 1% of the prediction.

NOTATION

E - quadratic deviation
f - Sigma function, in Eq. (2)
n - number of input variables in the neural network model
NH - number of neurons in the hidden layer
N.SETS - number of presentations of the data to the network
O_k - ouput from neuron k in the output layer
p - number of output variables in the neural network model
p_F . pressure in the feed line
p_P - pressure in the product line

p_W - pressure in the waste line
q - number of input variables in the network
Q_P - mass flow of the product;
Q_W - mass flow of the waste;
r - number of input/output pairs in the learning set
RMST -learning set sum of errors
RMSTT- test set sum of errors
R_P - abundance ratio of the product;
R_W - abundance ratio of the waste.
S_v - weighted sum of inputs to a neuron
$W_{u,v}$ - weight of variable i, in neuron j
yk - experimental output variable k

Greek symbols
α - separation factor
β - enrichment factor
γ - depleting factor
dU - separation power

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