CHEMICAL ENGINEERING TRANSACTIONS Volume 17, 2009
Editor Sauro Pierucci
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DOI: 10.3303/CET0917232

Design and Implementation of a Neural Network Based Soft Sensor to Infer Sulfur Content in a Brazilian Diesel Hydrotreating Unit

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The diesel hydrotreating (HDT) process in refining oil plants is a conversion process responsible for the specification of this product in oil industry. In this work, the objective was to estimate sulfur content in the outlet stream of the unit, using inferences based on heuristic modeling. Neural networks (NN) were used to correlate the sulfur content, measured offline in laboratories, with variables measured on-line (as temperature and flow rates) in the reaction section of the HDT unit. Historical data was loaded from Petrobras (Brazilian Oil Company) Duque de Caxias Refinery (REDUC) in Rio de Janeiro and treated in order to remove outliers and reduce dimensionality. After that, twenty-four different designs of neural networks were trained to find out the best fit to real data. The chosen neural network was implemented in the refinery's data storing and acquisition system. Very good predicitons of sulfur content were obtained indicating the use of this inference for advanced process control.

1. Introduction

The search for the maximization of light products from heavier petroleum and more stringent enviromental restrictions give remarkable importance to conversion processes of heavy oil fractions into more valuable lighter ones (Speight, 2004). At present, the hydrotreating (HDT) process plays a major role in refineries. In addition the monitoring of HDT units bring benefits such as energy savings, reduced off-specification products generation, less operational problems etc. However, analytical measurements of product quality variables may be expensive, unreliable and require long times. In this scenario, the real time monitoring of HDT units − specially of product sulfur content − based on inference models is justified.

Inference models employing easily measurable operational variables (secondary variables) may be developed, based on the hypothesis that variations in these secondary variables reflect variations in the primary (or target) ones. Neural Networks (NNs) are recommended for heuristic modeling strategies in which the process is represented based on the knowledge of experts and/or on process history data.

This contribution presents the develoment of a soft sensor based on NNs in which the sulfur content in a converted diesel product was the inferred variable and the flow rates, temperatures and pressure in the HDT unit were the secondary variables. Data from a

Please cite this article as: Salvatore L., De Souza Jr. M. and Campos M., (2009), Design and implementation of a neural network based soft-sensor to infer sulfur content in a brazilian diesel hydrotreating unit, Chemical Engineering Transactions, 17, 1389-1394
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HDT diesel unit located in Petrobras (Brazilian Oil Company) Duque de Caxias Refinery (REDUC), Brazil, were used for the study.

2. The HDT Process: Description and Data

A hydrotreating plant is composed by a reaction section – which includes a series of pre-heating furnaces, the reactors, the hydrogen flash system and the make-up compressor for hydrogen – and a stabilization section. In the present work, only the reaction section was focused because it is the most important one as the reactions and the major disturbances (related to feed and hydrogen flow rates) happen there. The diagram of this part of the unit can be seen in Figure 1.

Two reactors are employed in REDUC Refinery. The reactors are trickle bed ones as the inflow enters in gaseous and liquid phases, composing a triphasic system together with hydrogen and the catalyst solid bed. A quench system is used to control the temperature of the reactors. This is achieved with the injection of a hydrogen stream in the middle of catalytic beds. The yield products of this unit are finally directed to stabilization section, where all commercial specifications are adjusted.

A total of 13 (input) variables that influence the sulfur content in the diesel product (output variable) and that are are available on-line were chosen. The location of these measurements in shown in Figure 1 as follows: feed diesel flow rate (1); recycle (2) and make-up (3) hydrogen flow rates; temperature in the input stream to reactor 1 (4); hydrogen recycle for reactor 1 (5); temperature in the input stream to reactor 2 (6); hydrogen recycle for reactor 2 (7); temperature in the hydrogen recycle stream (8); temperature measurements in beds 1 and 2 of reactors 1 (9 and 10, respectively) and 2 (11 and 12, respectively) and partial hydrogen pressure in the unit (13).

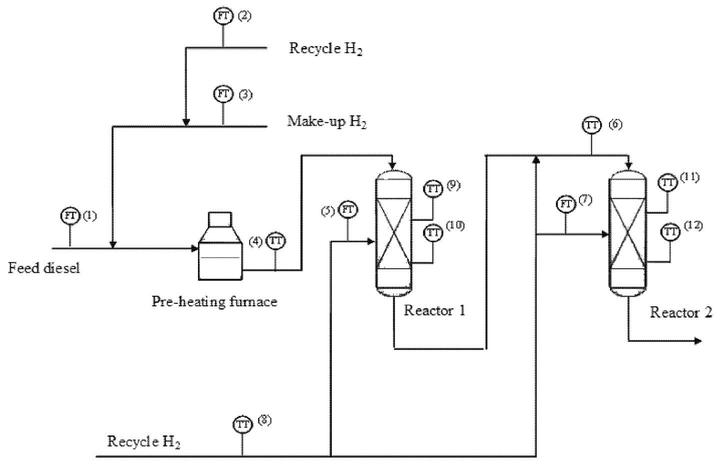

Figure 1 HDT Reaction Section

The period between Juny 2005 and June 2006 was chosen as historical database, being part of it illustrated in Figure 2. Daily laboratory analysis of sulfur content in the diesel product were available. In order to consider dynamic effects, all the input variables were collected at previous times (at 2 h; 2 ½ h; 3 h and 3 ½ h earlier) in relation to the time when the sample to analyse the sulfur content in the output of the unit was taken (Salvatore, 2008). These data were available in the PI System™ of the refinery.

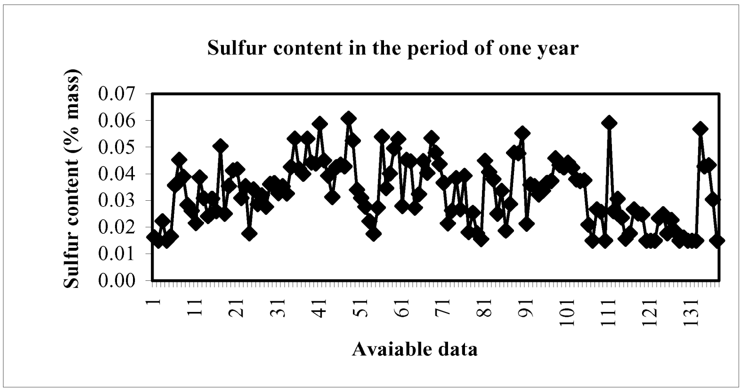

Figure 2 Historical database

Because of these delayed measurements, the number of inputs to the models built up to four times (from 13 to 52). This increase in the number of inputs implies a need for more data in order to avoid overfiting of the NNs. This − together with the fact that the input variables may not be independent among themselves − motivated the application of dimensionality reduction techniques, as presented ahead in this text.

3. Development of the NNs

NNs were applied as an estimator of product quality based. The module STATISTICA NEURAL NETWORKS (SNN) of the program Statistica™ version 6.0 was utilized.
Multilayer Perceptron (MLP) and Radial Base Function (RBF) networks were tested. These nets have a multilayer topology with feedforward connections; both types have linear neurons in the input and output layers. The hidden units have sigmoidal activation functions in the MLP and radial functions in the RBF networks. MLP networks are trained by supervisioned (typically modified backpropagation) methods, while RBF networks are trained using both unsupervisioned (for the location of the centers and establishment of the deviation of the radial units) and supervisioned (linear optimization for the weights between the hidden and output layers) methods. Both paradigms are very well documented in the literature (Haykin, 1999). Linear NNs were also used here for comparison purpose, these NNs have only two layers with linear units.
Before using the data for training the NNs, outliers were discarded (Salvatore, 2008). The amount of data was increased using spline interpolation. This allowed the amount of data to be increased by a factor of 10, rendering 1291 patterns (2/3 randomly used for training and 1/3, for validation).
The models were selected on the basis of the S.D. ratio. The S.D. ratio is obtained by dividing the standard-deviation obtained by the difference between the predicted values

and the individual target values by the standard deviation of the data. Models with S.D. ratio between 1.0 and a little less than 1.0 achieve bad to reasonable predictions, but models with S.D. ratio between 0.2 and 0.1 usually show very good performances (Salvatore, 2008). Sensitivity analysis were also perfomed with the trained NNs in order to discard variables. The procedure treated each input variable as if it wasn't available to analyses, substituting it by its average value. Dividing the total network error, when the variable was 'unavailable', by the total network error, when the variable values were used as input values, resulted in a ratio that would have a value bigger than 1.0 if the variable contributed to the resolution of the problem.

For each group of inputs tested, one hundred NN were trained. The best MLP, RBF and MLP NNs (one of each) were retained for each group based on the S.D. ratio, as shown in Table 1, which will be fully described in item 4.

Group I comprises nets trained using all the 52 inputs. *Group II* contains the nets that were obtained after the use of pruning techniques, based on the sensitivity procedure described above. *Group III* contains the NNs obtained after the application of *feature selection techniques*, like successive inclusion (*forward*) or exclusion (*backward*) of variables. *Group IV* includes NNs trained after the application of a *dimensionality reduction* (or *feature extraction*) procedure based on *dynamic principal component* (DPCA) analysis, according to a methodology proposed by Ku, Storer and Georgakis (1995). Additionally, a new set of inputs was chosen based on the location of the measurements. For the variables whose measurements were proceeded far from the sampling location of the diesel output stream, only two delayed measurements were used (at -3 and -3 ½ h). With this strategy, the number of inputs was reduced to 31. These NNs are named here *'Improved Heuristics´* and they belong to *Group IV* or *V*, wheter *pruning* is used or not. A more detailed discussion is found in Salvatore (2008).

4. Results and Discussions

Table 1 presents the results for the best NNs for each group. In that table, the description of the NN follows the order: type, number of neurons in the input, hidden and output (always 1 here) layer. The NNs were compared according to the smaller S.D. ratio, bigger R^2 and smaller number of paramters.

The analysis of Table 1 shows that the RBF NNs present an excessive number of parameters. So, they were not chosen as soft sensors. Continuing the evaluation of the models, it can be seen that the NN 6, an MLP, would be the best option after the RBFs, if the S.D. ratio were the only criterium taken into account. However, it can be seen that this NN is not adequate, because its number of parameters (817) is high, considering the number of training patterns used (860).

The NNs in *Group IV* used 9 principal components, defined through the methodology of Ku, Storer and Georgakis (1995). However, these NNs did not present a good performance, what may be explained by the fact that DPCA is a linear technique and one of the most distinguished characteristics of the HDT process is its nonlinearity. A complete discussion can be found in Salvatore (2008).

Table 1: Results for each trained NN

NN	Group	Description	S.D. ratio (Validation)	R^2	Number of Parameters
1		RBF 52-318-1	0,072258	0.99477	17173
2	*I*	Linear 52-1	0.657589	0.56806	52
3		MLP 52-18-1	0.129320	0.98329	973
4		RBF 47-323-1	0.071996	0.99481	15828
5	*II*	Linear 30-1	0.751090	0.43586	30
6		MLP 46-17-1	0.121310	0.98528	817
7		RBF 42-303-1	0.090881	0.99174	13333
8	*III*	Linear 42-1	0.747104	0.44219	42
9		MLP 42-17-1	0.161896	0.97389	749
10		RBF 9-323-1	0.085875	0.99265	3554
11	*IV*	Linear 9-1	0.839976	0.29453	9
12		MLP 9-10-1	0.431394	0.81462	111
13		RBF 31-323-1	0.041674	0.99826	10660
14	*V*	Linear 31-1	0.802164	0.35655	31
15		MLP 31-17-1	0.154924	0.97599	562
16		RBF 31-307-1	0.058699	0.99655	10132
17	*VI*	Linear 25-1	0.804042	0.35399	25
18		MLP 29-15-1	0.212412	0.95593	466
19		RBF 33-291-1	0.018809	0.99964	10186
20	*VII*	Linear 33-1	0.019963	0.99960	33
21		MLP 33-7-1	0.022242	0.99950	246
22		RBF 30-47-1	0.192327	0.96301	1505
23	*VIII*	Linear 25-1	0.020141	0.99959	25
24		MLP 10-4-1	0.025780	0.99934	49

Trying to further improve the results, a new model based on NN was proposed. NN 15 was chosen for being the most parsimonious one, that presented a satisfactory result in terms of S.D. ratio and R^2 correlation, while still attending the heuristic criteria, which considered that the dynamics of the HDT process demanded three to four hour delays between the inputs and the output variable. In this new approach, two delayed samples of sulfur content were used as inputs together with the other 31 inputs of NN 15. The past sulfur content data were available in the PI System™.

Analogously to what was proceeded previously, the nets were tested without (*Group VII*) and with *pruning* (*Group VIII*) as shown in Table 1. As can be seen, the inclusion of delayed sulfur data greatly improved the performance of the NNs. NN 21 and 24 present the best results when the 3 characteristics are analysed together. Even though, NN 21 present more parameters, it can still be considered for industrial implementation, once the proportion patterns/parameters is acceptable. It can also be seen that in this case the linear NNs presented good performances. However, the linear models were not implemented, because the HDT process is highly nonlinear and the MLP NNs are expected to render a more robust behavior in such a case.

NN 21 was implemented as soft sensor in the in the PI System™ of the refinery to infer the sulfur content in real time. Figure 3 shows the inference and real laboratory data for a three week window. It can be seen that the predictions of the NN follow very well the real data. Presently, this NN is still being used as a soft sensor and it is also aimed to use it in the advanced control system that will be implemented in the HDT unit.

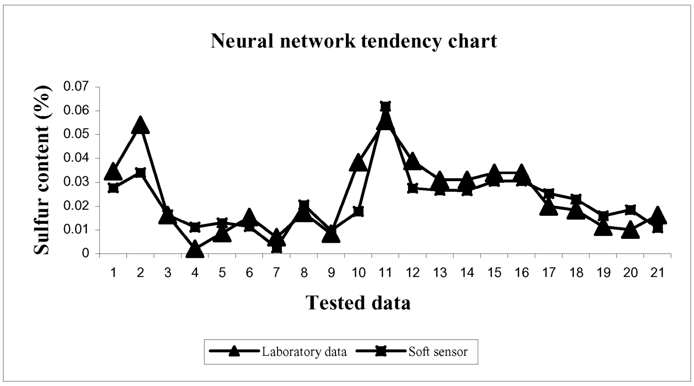

Figure 3: Results of the soft-sensor implemented in the refinery

5. Conclusions

The application of industrial knowledge together with advanced optimization and statistic softwares produced a very effective NN soft sensor to infer sulfur content in the HDT unit. The MLP reveaeled itself as the best NN;. Besides presenting good predictive ability, the compactness of the MLP eased its implementation in the PI System™ and demanded very low computational effort. Tests were performed in which it was verified that the execution intervals of the soft sensor can be lowered down to 1s. So, it is expected that this tool may be used both for monitoring and advanced process control.

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ACKNOWLEDGMENTS - This work was sponsored by 'Brazilian Research and Projects Financing Agency' (FINEP) and PETROBRAS (Grant 01.04.0902.00).