An Expert System to Improve the Energy Efficiency of the Reaction Zone of a Petrochemical Plant

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Abstract. Energy is the most important cost factor in the petrochemical industry. Thus, energy efficiency improvement is an important way to reduce these costs and to increase predictable earnings, especially in times of high energy price volatility. This work describes the development of an expert system for the improvement of this efficiency of the reaction zone of a petrochemical plant. This system has been developed after a data mining process of the variables registered in the plant. Besides, a kernel of neural networks has been embedded in the expert system. A graphical environment integrating the proposed system was developed in order to test the system. With the application of the expert system, the energy saving on the applied zone would have been about 20%.

Keywords: Energy efficiency, petrochemical plant, data mining, expert system.

1   Introduction

Expert systems are being successfully applied for the realization of diverse tasks (interpretation, prediction, diagnosis, design, planning, instruction, control, etc.) in multiple fields such as medicine, geology, chemistry, engineering, etc. Such applications are very affective in situations when the domain expert is not readily available [1]. There are diverse problems which need to be solved in the real world and they are difficult to solve by the expert at the moment of carrying out his work. Thus, the expert systems, and specifically the decision systems, become prolific in many fields [2]. On the other hand, data mining (or the analysis step of the knowledge discovery in databases) [3] is a discipline intimately related to expert system and which makes it possible to extract the necessary knowledge for them.

The energy efficiency of plants is an important issue in any type of business but particularly in the chemical industry. Not only is it important in order to reduce costs, but also it is necessary even more as a means of reducing the amount of fuel that gets wasted, thereby improving productivity, ensuring better product quality, and generally increasing profits. At the same time, and as an added advantage of this optimization, keeping energy efficiency in petrochemical plants helps to reduce climate change.

Besides, in chemical industry, one of the complex problems for the control of which a computational intelligent approach has sense, is a crude oil distillation unit.

In a crude distillation process, the first objective is to perform an entire process optimization including high production rate with a required product quality by searching an optimal operating condition of the operating variables. In the previous decade, there was considerable research concerning the optimization of crude distillation process. In [4], the optimal feed location on both the main column and stabilizer is obtained by solving rigorous "a priori" models and mixed integer nonlinear programming. The sensitivity to small variations in feed composition is studied in [5]. Julka et al. propose in a two-part article [6][7] a unified framework for modeling, monitoring and management of supply chain from crude selection and purchase to crude refining. In addition to analytical non-linear models, computational intelligence techniques such as neural networks [8] and genetic algorithms [9] are used for the same purpose. In particular, neural networks have been used for modeling and estimation of processes in petrochemical and refineries [10][11][12]. ´

There is a part of the crude oil distillation called the platforming unit. The objective of present study is focused with this part. This zone is constituted of two subunits: the catalytic reforming or reaction unit and the distillation unit or train distillation. The expert system is focused on optimizing the production rate of the reaction unit.


2   The Petrochemical Plant

Refineries are composed of several operating units that are used to separate fractions, improve the quality of these fractions and increase the production of higher valued products like gasoline, jet fuel, diesel oil and home heating oil. The function of the refinery is to separate the crude oil into many kinds of petroleum products. This work pays special attention to Platforming Unit. This unit is constituted of two basic units: The catalytic reforming or reaction unit and the distillation unit or train distillation.

The catalytic reforming of naphtha is an important refining process that seeks to improve the octane number of gasoline due to a conversion to paraffins and naphthenes in aromatics. The feed to the naphtha reformer is a crude oil fraction from the refinery crude unit with a boiling range between 100°C and 180°C. This process is adiabatically carried out at high temperatures, building up gasoline with a high octane number, LPG, in three reformers: hydrogen, fuel gas and coke. The coke deposits on the spent catalyst surface causing its deactivation. To recover its activation, the catalyst with coke is regenerated after certain running time.

In the first reactor, the major reactions such as dehydrogenation of naphthenes are endothermic and very fast, causing a very sharp temperature drop. For this reason, this process is designed using a set of multiple reactors. Heaters between the reactors allow an adequate reaction temperature level to maintain the catalyst operation.

This process is performed in three different distillation columns (Fig. 1). The separator liquid and a stream, called aromatic LPG from the external platforming unit, feed off the first column, the debutanizer column. This column fractionates the input into two basic products: butane, to the top of the column and a high hydrocarbon flow, also called platformer, to the bottom of the column. Platformer feeds off the

debenzenizer, the second distillation unit. Its goal is to obtain a light aromatic flow to the top free to the high hydrocarbon. This stream is fed off the third distillation column that produces benzene and toluene. Benzene and toluene are the important products to the plant. The products are sent to the Morphylane Unit and, the bottom product to the second column and the top product to the third column, are stored up or sent to the other units of the refinery.
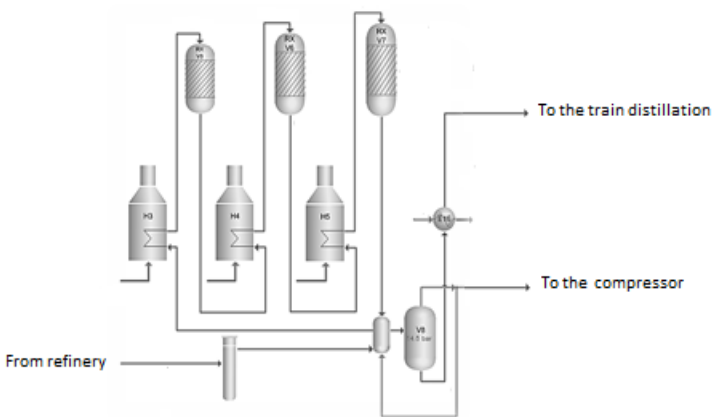
Fig. 1. Flow diagram of the catalytic reforming plant

As the platforming unit is one of the critical and important unit operations for the petroleum industry, the goal is to achieve a well-controlled and stable system, high production rate and product quality as well as low operating cost for the economic consideration. For this reason, the attention has been paid to this unit to improve product rate, efficiency and quality assurance in petroleum industry in recent years. Our work of improving of the energy efficiency is focused in the first zone of the platforming unit: the reaction zone.

3 Data Mining Process

First of all, in order to design of the expert system we carried out a data mining process of the variables registered in the reaction zone of the petrochemical plant. Thus, this type of processes requires, first of all, a selection of the sample set and, later, a preprocessing where the data are analyzed, filtered, and formatted [13][14]. The frequency of registering of the plant was hourly, but the quality of the product is analyzed only once a day. The time interval of the samples of data that we had was from January 2009 to May 2010. So, the total sample contained 12149 records corresponding to the set of variables of the plant in hourly register. The parameters of the reaction zone of the plant, which we used as inputs for our expert system, are described in Table 1.

Table 1. Main variables of the reaction zone of the plant

Variable name	Meaning
WAIPTF (C)	The variable that measure the catalysts Deterioration
TPRIN PPPV7 (C)	The input PPV7 reactor's temperature.
TPROUT PPV6 (C)	The output PPV6 reactor's temperature.
TPROUT PPV5 (C)	The output PPV5 reactor's temperature.
TPRIN PPV7 (C)	The input PPV7 reactor's temperature.
TPRIN PPV6 (C)	The input PPV6 reactor's temperature.
TPRIN PPV5 (C)	The input PPV5 reactor's temperature.
CSMFGPPH3 (m3/h)	The fuel gas PPH3 heater's consumption.
CSMFGPPH4 (m3/h)	The fuel gas PPH4 heater's consumption.
CSMFGPPH3 (m3/h)	The fuel gas PPH5 heater's consumption.
PTFINFLOW (m3/h)	The platforming input flow.
P PPV8 (bar)	The PPV8 product separator pressure.
TPROOM (C)	The room temperature.
DENRECGAS (Kg/(N*m3))	The recycle gas density. This variable manitain the PPPV8 brought under control.
TPRPPV567 (C)	The temperature increase between the three reactors.

In the first step of preprocessing, 120 outliers corresponding to the days where the plant did not have a usual operation were filtered and deleted from the training sample. Besides, the resulting sample was filtered on the basis of a quality requirement (Concretely that the limit of the level of impurities in the distillate satisfies a determining conditions). Thus, 2747 registers were filtered. Thus, after the selection and preprocessing processes, the resulting sample had 9282 records.

In order to quantify the objective of our mining, in the phase of transformation we added to each register of the sample an indicator of the energy efficient of the reaction zone:

$$EEI_{REACTION} = \frac{\sum_{i=3}^{5} CSMFGPPH_i}{PTFINFLOW} \qquad (1)$$

As a first algorithm in the data mining modeling, we applied a discriminant analysis [13][14] to the set sample. This type of analysis is used for classification and prediction. Thus, this model tries to predict, on the basis of one or more predictor, or independent variables, whether an individual or any other subject can be placed in a particular category of a categorical-dependent variable. Our aim with this analysis was to study the influence of the variables of the zone in the EEI parameter as well as the grade of importance of each of these variables.

Thus, the result of this analysis was a discretization and separation of the five classes of *EEI_Reaction* through a linear combination of the input parameters. The model evaluation was performed first using ten-fold cross validation in the training sample. Later, a new validation by means of the testing sample was done. This kind of

evaluation was selected to train the algorithms using the entire testing data set and obtain a more precise model.

The result of the discriminant analysis was two canonical functions (named *Function1* and *Function2*). *Function1* covered 96.8% of the variance, and *Function2* covered only an additional 1.5%. So, and in view of this difference in percentage, we use only *Function1* as a guide of *EEI_Reaction*.

Using the normalized variables, the discriminant analysis offers a structure matrix that allows building the discriminant functions from discriminating variables, without using the canonical form. From now on, the N prefix indicates a normalized attribute. Variables are ordered by the absolute size of correlation within functions. Using the normalized variables, and by weighing up the high percentage of variance covered by *Function1*, the plant energy efficiency will be improved by means of the new attribute defined in (2).

$$F = 0.28 * N\_CSMFGPPH5 + 0.27 * N\_CSMFGPPH3 - 0.27 * N\_PTFINFLOW - 0.213 * N\_P\_PPV8 + 0.009 * N\_DENRECGAS + 0.160 * N\_CSMFGPPH4 + 0.160 * N\_TPROOM + 0.013 * N\_TPRPPV567 \tag{2}$$

Thus, this function marks the way that follows the operating points registered for the plant. As observed in Fig. 2, low values of *F* (specifically below -0.6) guarantee, in a high percentage, low consumption (an *EEI_Reaction* that is between 15 and 36) with regard to the platforming input flow. This resulting function *F* would be used as a guide and an input parameter in the optimization algorithm based on neural networks [13][14].

4   Expert System Based on Neural Networks

In order to carry out a system for the optimization of the energy efficiency of the operation points in the plant, an expert system based on a neural network kernel was developed. The system combines an algorithm based on the historical data of working environment of the plant, and an artificial neural network module for additional interpolations of new work environments. Therefore, in order to take decisions this solution uses a combination of the known conditions given in the past in the plant and the capacity of the neural network to generate new interpolated conditions when it is necessary.

We developed an application programmed in C++ to work on Microsoft Windows, where we integrated our expert system. This application makes it possible to test the system and to visualize its results. In this section of the work, we will show screenshots of various windows to explain the system and to show its results. The environment includes the following working areas:

-    The value of different parameters for the operating point to optimize (distinguishing between controllable and not controllable variables, depending if they are variables whose value is adjustable by the operator of the plant or not). Besides, editable values beside each variable indicate the percent value of each variable that can be moved by the operator in each iteration.

- A plot in which you can observe, for each of the various operating point of the historic, its *EEI_Reaction* and *F*.
- The configuration of the ratio of improvement that the neural networks applied to the operation point (the X-axis corresponds to *F* offset and the Y-axis corresponds to *EEI_Reaction* and a ratio by which these values are multiplied).
- A historic text showing the evolution of different variables along the process of iterations of the algorithm to optimize the energy efficiency.
- A set of buttons to carry out the execution and test the hybrid model for a particular operating point.
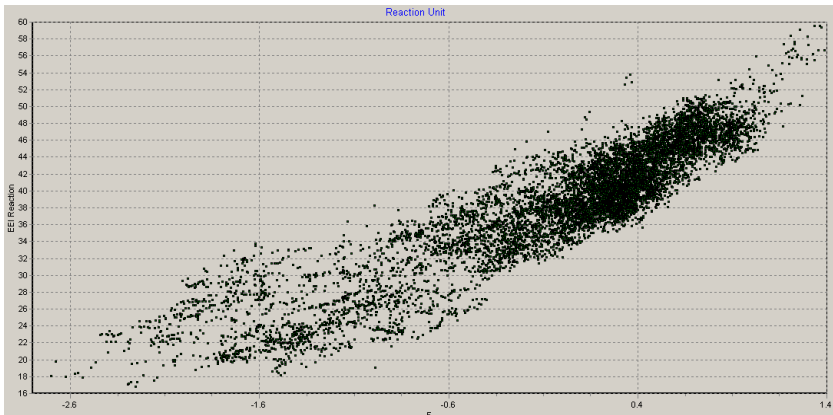
Fig. 2. Representation of the operations points with respect to *EEI_Reaction* and *F*

On the other hand, the algorithm of the expert system works in the following way once that is selected the operation point that is necessary to optimize:

1. First of all, it is filtered the sample by the environmental conditions in the actions of the operator of the plant (Selecting those registers whose values are out of a maximum percentage in which the values of the variables can be moved in each one of the iterations). In this respect, we distinguished between the conditions of the not controllable variables (those conditions for the starting point of work you want to optimize and which shall not be violated throughout the optimization process from that point) and the conditions set for the controllable variables (valid for the point which is currently being processed). The result of this filtering process is shown in Fig. 3.

2. With the *Start* button is activated the optimization process. This process consists of a loop which in each iteration is searched for a point (from the set of points of the historical) which meets the environmental conditions marked (described in the point 3 of the algorithm) that has the lowest energy. Thus, each one of these iterations improves the energy conditions since the previous point and shows the operator of the plant how carry out that improvement.

3. When it is not possible to improve the energy index of the current point using the historical register of the plant and meeting the conditions of iteration, the previous

loop stops. At this point a neural network module is fired in order to improve the energy index. This module generates, by means an interpolation process, a new working point, fulfilling the conditions set for improving the energy index variables that point. (This improvement consists of a shift of both the energy index as the function F -described in section 3-).

4. In this state, you can shoot again the optimization process to search, from this new point generated by interpolation, historical points that improve the *EEI_Reaction* to meet the conditions for the variables configured. Thus, once a new interpolated point is generated, the steps 2 and 3 can be executed by the user iteratively, until that operator of the plan reaches the desired improvement in the *EEI_Reaction*. The objective is to get the operation point with less *EEI_Reaction* of the resulting of the step 1 (as it is shown in Fig. 4).

The scheme of neural networks used for our system is shown in Fig. 5. It consists of a sequential structure of networks. Each network has got as inputs the not controllable variables (*N_PTFINFLOW, N_DENRECGAS, N_TPROOM, N_TPRPPV567*) as well as the two parameters that guide the energy efficiency (*F* and *EEI_Reaction*). The neural network 1 generates a value for the most important controllable variable (*N_P_PPV8*). The generated output is taken additionally as input by the neural network 2 and so on. The order of importance of the variables generated is given by the weight in equation (2). With this scheme, we get a less error in the adjustment for the most important variables.

The configuration of the neural networks was a Backpropagation network and they had a single hidden layer with 6 neurons for the case of the first network and 8 in the other networks. For the training process of these networks we used the 80% of the points of historical work as training patterns and 20% as validation patterns. The results reached in the adjustments of the neural networks were respectively 96.58%, 96.33%, 99.75% and 99.74%.
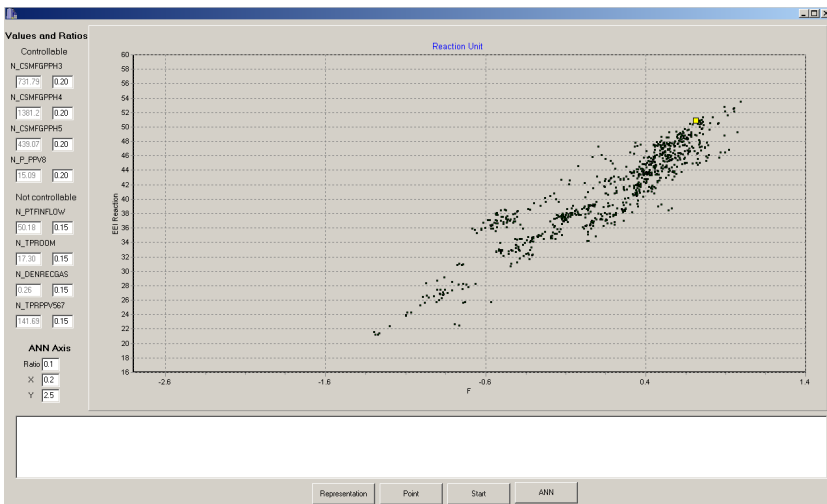
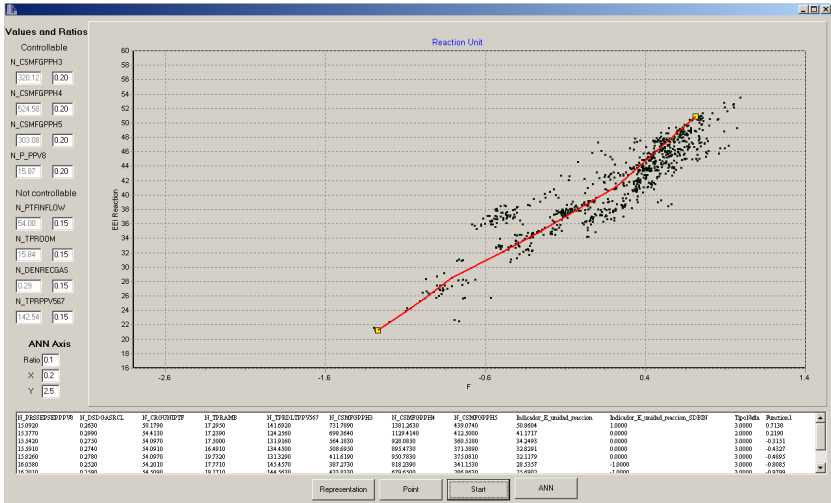**Fig. 3.** Representation of the operation points for the current work conditions

Fig. 4. Result after the optimization process carried out by the system
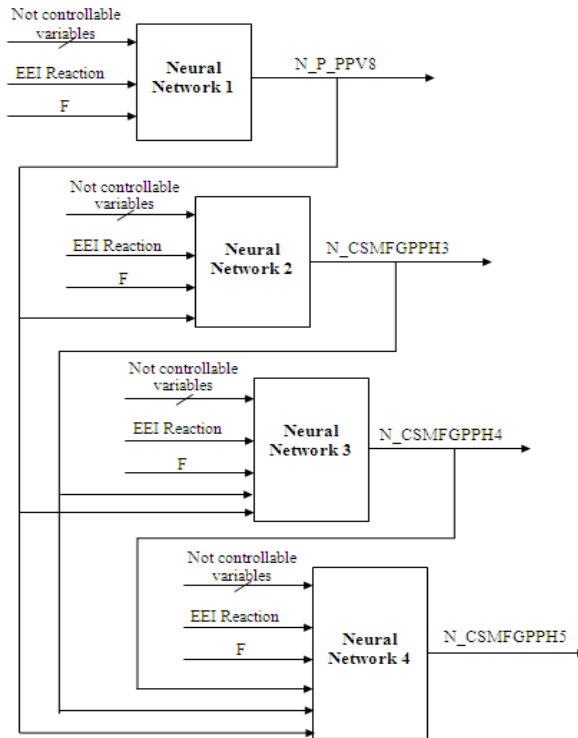

Fig. 5. Scheme of neural networks of the expert system

5   Results and Conclusions

For the quantification of the results, we generated a methodology in order to carry out a measurement of the overall improvement that would have been reached with our system for the total number of registers occurred in the past. Thus, the objective of the methodology was to apply our expert system to all the points of the sample set calculating the improvement percentage for each point and to calculate the mean improvement for the entire sample. Thus, if the expert system becomes applied on the operation points registered in the past, the energy efficiency of the zone (*EEI_Reaction*) would have improved 18.52%. This result is very good taking into account that a lot of operating points were in the range of [15,40] in their *EEI_Reaction* value and therefore, the scope of improvement was less. Thus, in an analysis of the results, we can observe as the improvement was 26.12% for those operating points with *EEI_Reaction* higher that 45 (some operating points reached an improvement of 40%).

As a conclusion of this work, it is necessary to emphasize that we have developed a tested expert system based on a module of neural networks for the optimization of the consumption of a part of a petrochemical plant. The energy efficiency is an important task that at the same time that it improves the consumption of the plant, it helps to reduce climate change. The expert system has been developed after a data mining process. It is integrated by an algorithm which uses the information relative to the parameters registered for the plant, and other hand, a scheme of neural networks for optimizing additional future operation points. Thus, this algorithm makes it possible for the operator to guide its work with a security in energy efficiency issues. This methodology for the optimization, which is the main contribution of our work, has got two advantages:

- The system is working on real conditions of operation. Thus, the use of an interpolation algorithm as neural networks is only for linking the operation point in the present with operation points that had already happened in the past. This fact ensures results that are not only theoretical but also eminently practical.
- The system can be constantly improved by means of the use of the operation points occurred in the future which can be used to adjust the neural networks.

Currently, we are working to apply the expert system to the whole plant. Besides, our objective is to integrate the expert system in the SCADA monitoring system.

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