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Soft-Sensor for Estimation of Gasoline Octane Number in Platforming Processes with Adaptive Neuro-Fuzzy Inference Systems (ANFIS)

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Abstract**—**Gasoline Octane Number is the standard measure of the anti-knock properties of a motor in platforming processes, that is one of the important unit operations for oil refineries and can be determined with online measurement or use CFR (Cooperative Fuel Research) engines. Online measurements of the Octane number can be done using direct octane number analyzers, that it is too expensive, so we have to find feasible analyzer, like ANFIS estimators.

ANFIS is the systems that neural network incorporated in fuzzy systems, using data automatically by learning algorithms of NNs. ANFIS constructs an input-output mapping based both on human knowledge and on generated input-output data pairs.

In this research, 31 industrial data sets are used (21 data for training and the rest of the data used for generalization). Results show that, according to this simulation, hybrid method training algorithm in ANFIS has good agreements between industrial data and simulated results.

Keywords**—**Adaptive Neuro-Fuzzy Inference Systems, Gasoline Octane Number, Soft-sensor, Catalytic Naphtha Reforming

I. Introduction

THE inferential sensing technology was originally developed to improve the control of chemical and biological processes [1].Inferential sensing is difficult to measure process parameters to be inferred from other easily made measurements [2]. All inferential sensors are based on an inferential modeling module that represents the dynamics between the inputs, or easily measurable variables, and the output, or undetectable variables.

Listed below are some commonly used approaches for the development of the inferential modeling module:

_ Physical model
_ Neural network
_ Fuzzy logic
_ Adaptive neuro-fuzzy inference system

Despite considerable success in chemical and biological engineering, the inferential sensing and control techniques have not been popularly used in building automation. Some researchers began to investigate the benefit of incorporating the inferential sensing technique with conventional building control schemes [6].

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II. Catalytic Naphtha Reforming Process

Catalytic reforming is a process whereby light petroleum distillates (naphtha) are contacted with a platinum-containing catalyst at elevated temperatures and hydrogen pressures ranging from 345 to 3,450 kPa (50–500 psig) for the purpose of raising the octane number of the hydrocarbon feed stream. The low octane, paraffin-rich naphtha feed is converted to a high-octane liquid product that is rich in aromatic compounds.

Hydrogen and other light hydrocarbons are also produced as reaction by-products. In addition to the use of reformate as a blending component of motor fuels, it is also a primary source of aromatics used in the petrochemical industry [3].

Catalytic reforming processes were improved by introducing bimetallic catalysts. These catalysts allowed lower pressure, higher severity operation: 1,380–2,070 kPa (200–300 psig), at 95–98 octane with typical cycle lengths of one year. Cyclic reforming was developed to allow operation at increased severity. [4]

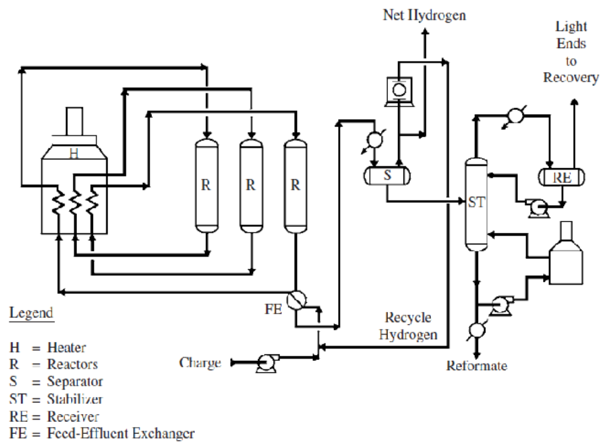

Fig. 1 Catalytic Naphtha Reforming process [5]

III. ANFIS

The aim is to use the ANFIS methodology, a hybrid structure, in the estimation of platformate Octane number using Reactor temperature, H_2/Hc Ratio and Product Separator Temp in Catalytic Naphtha Reforming Unit. The performance of the ANFIS estimator is compared with industrial data.

In this paper, the design of ANFIS architecture for the estimation Purposes will be explained.

As previously stated, ANFIS is an adaptive network that is functionally equivalent to fuzzy inference system (Jang 1993), and referred in literature as “adaptive network based fuzzy inference system” or “adaptive neuro fuzzy inference system”. In this section architecture of ANFIS will be presented.

A. ANFIS Architecture

In ANFIS, Takagi-Sugeno type fuzzy inference system is used. The output of each rule can be a linear combination of input variables plus a constant term or can be only a constant term. The final output is the weighted average of each rule's output. Basic ANFIS architecture that has two inputs x and y and one output z is shown in Figure 2. The rule base contains two Takagi-Sugeno if-then rules as follows:

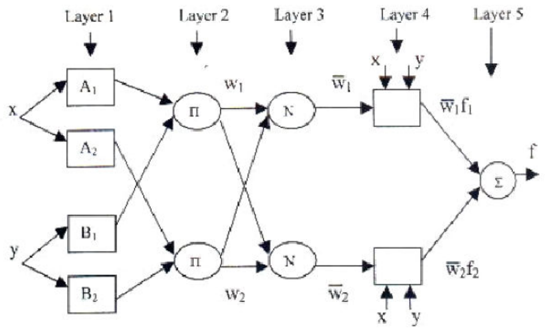

Fig. 2 Basic structure of ANFIS

The node functions in the same layer are the same as described below:

Layer 1: Every node i in this layer is a square node with a node function as:

$$O_{1,i} = \mu_{A_i}(x), \quad for\ i = 1,2$$
$$O_{1,i} = \mu_{B_i - 2}(y), \quad for\ i = 1,2$$

Where x is the input to node i, and A_i (or B_{i-2}) is a linguistic label (such as "small" or "large") associated with this node. In other words, $O_{1,i}$ is the membership grade of a fuzzy set A and it specifies the degree to which the given input x satisfies the quantifier A . The membership function for A can be any appropriate membership function, such as the Triangular or Gaussian. When the parameters of membership function change, chosen membership function varies accordingly, thus exhibiting various forms of membership function for a fuzzy set A. Parameters in this layer are referred to as "premise parameters".

Layer 2: Every node in this layer is a fixed node labeled as Π, whose output is the product of all incoming signals:

$$O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y), \quad i = 1,2$$

Each node output represents the firing strength of a fuzzy rule.

Layer 3: Every node in this layer is a fixed node labeled N. The *i*th node calculates the ratio of the rule's firing strength to the sum of all rules' firing strengths:

$$O_{3,i} = \overline{w}_i = w_i / (w_1 + w_2), \quad i = 1,2$$

Outputs of this layer are called "normalized firing strengths".

Layer 4: Every node *i* in this layer is an adaptive node with a node function as:

$$O_{4,i} = \overline{w}_i f_i = \overline{w}_i (p_i x + q_i y + r_i)$$

Where w_i is a normalized firing strength from layer 3 $\{p_i, q_i, r_i\}$ is the parameter set of this node. Parameters in this layer are referred to as "consequent parameters".

Layer 5: The single node in this layer is a fixed node labeled Σ that computes the overall output as the summation of all incoming signals:

$$overall\ output = O_{5,i} = \sum_i \overline{w}_i f_i = \frac{\sum_i w_i f}{\sum_i w_i}$$

Thus an adaptive network, which is functionally equivalent to the Takagi- Sugeno type fuzzy inference system, has been constructed. Other example of ANFIS with nine rules can be shown in Figure 3. Three membership functions are associated with each input, so the input space partitioned into nine fuzzy subspaces. The premise part of a rule describes a fuzzy subspace, while the consequent part specifies the output within this fuzzy subspace.

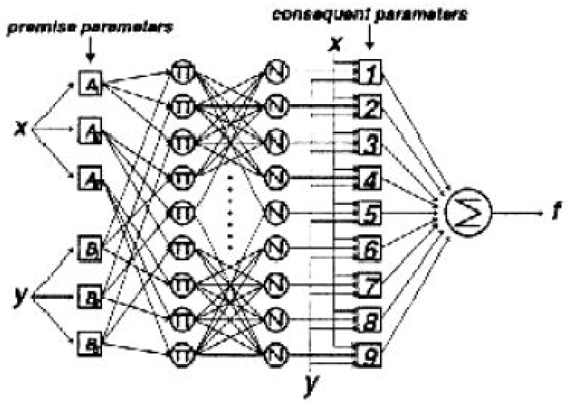

Fig. 3 ANFIS Architecture with nine rules

B. ANFIS learning algorithm

From the proposed ANFIS architecture (Fig. 3), the output f can be defined as:

$$f = \frac{w_1}{w_1 + w_2} f_1 + \frac{w_2}{w_1 + w_2} f_2$$
$$f = \overline{w}_1 (p_1 x + q_1 y + r_1) + \overline{w}_2 (p_2 x + q_2 y + r_2)$$
$$f = (\overline{w}_1 x) p_1 + (\overline{w}_1 y) q_1 + (\overline{w}_1) r_1 + (\overline{w}_2 x) p_2 + (\overline{w}_2 y) q_2 + (\overline{w}_2) r_2$$

Where p_1 , q_1 , r_1 , p_2 , q_2 and r_2 are the linear consequent parameters. The methods for updating the parameters are listed as below:

1. *Gradient decent only*: All parameters are updated by gradient decent backpropagation.
2. *Gradient decent and One pass of Least Square Estimates (LSE)*: The LSE is applied only once at the very beginning to get the initial values of the consequent parameters and then the gradient descent takes over to update all parameters.
3. *Gradient and LSE*: This is the hybrid learning rule.Since the hybrid learning approach converges much faster by reducing search space dimensions than the original backpropagation method, it is more desirable. In the forward pass of the hybrid learning, node outputs go forward until layer 4 and the consequent parameters are identified with the least square method. In the backward pass, the error rates propagate

backward and the premise parameters are updated by gradient descent.

IV. DESIGN OF ANFIS

The basic idea behind the neuro-adaptive learning techniques is very simple. These techniques provide a method for the fuzzy modeling procedure to learn information about data set, in order to compute the membership function parameters that best allow the associated fuzzy inference system to track the given input-output data. ANFIS constructs an input-output mapping based on both human knowledge (in the form of fuzzy if-then rules) and simulated input output data pairs. It serves as a basis for building the set of fuzzy if-then rules with appropriate membership functions to generate the input output pairs. The parameters associated with the membership functions are open to change through the learning process. The computation of these parameters (or their adjustment) is facilitated by a gradient vector, which provides a measure of how well the ANFIS is modeling the input output data for a given parameter set.

ANFIS can be used in modeling, estimating and controlling studies in chemical engineering processes similar to other artificial intelligence methods such as NNs and Fuzzy Logic (FL). In this work, the designed ANFIS is utilized as an estimator. Estimation is done for platformate Octane number using Reactor temperature, H_2/Hc Ratio and Product Separator Temp in Catalytic Naphtha Reforming Unit.

A. ANFIS as an Estimator

ANFIS can be used for the estimation of some dependent variables in chemical process. The designed ANFIS estimator is used to infer the platformate Octane number using Reactor temperature,H_2/Hc Ratio and Product Separator Temp in Catalytic Naphtha Reforming Unit .Estimation scheme is shown in Figure 1. In estimator design process, different ANFISs are constructed and trained to find the architecture that gives the best performance as an estimator. In order to design an estimator, first, training data sets should be generated to train the estimator networks. These data sets consist of estimator inputs and desired output values. They are produced from the process input output data. Since, ANFIS is a data processing method, it is important that the input-output data must be within the sufficient operational range including the maximum and minimum values for both input and output variables of the system. If this is not provided, estimator performance cannot be guaranteed and thus the designed estimator will not be accurate. Having generated the training data, estimators that have different architectures are trained with the obtained data sets.

Performances of the trained estimators are evaluated with model simulations and best estimator architecture is obtained. These simulations are made to verify and to generalize the ANFIS structures. Verification is done to show how good the estimator structure learned the given training data. This is carried out by simulating the column models with specific initial process inputs used in obtaining training data sets. Generalization capabilities of the estimators are found with other simulations in which input process variables are in operational range but not used in training data formation.

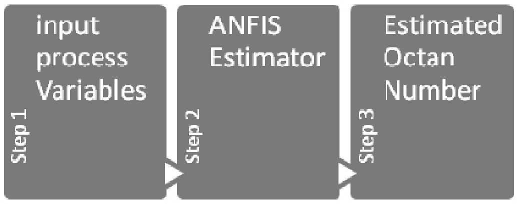

Fig. 4 Estimation using ANFIS estimator

ANFIS estimator design consists of two parts: constructing and training. In constructing part, structure parameters are determined. These are type and number of input Membership Functions (MFs), and type of output MF. Any of several MFs such as Triangular, Trapezoidal and Gaussian can be used as an input MF. Frequently used MFs in literature are the Triangular and Gaussian. For this reason, they are chosen as input MF type in this study. Number of MFs on each input can be chosen as 3, 5, and 7 to define the linguistic labels significantly. Effective partition of the input space is important and it can decrease the rule number and thus increase the speed in both learning and application phase. Output MFs can be either a constant or in linear form. Both of these two forms are used for the output MF in this study. Having described the number and type of input MFs, the estimator rule base is constituted. Since, there is no standard method to utilize the expert knowledge; automatic rule generation (grid partition) method is usually preferred (Castillo and Melin 2000).According to this method, for instance, an ANFIS model with two inputs and three MFs on each input would result in 3^2=9 Takagi-Sugeno fuzzy if-then rules automatically. Although this method can require much computational knowledge especially in systems that have to be defined with many inputs, it is used in this study due to advantage of MATLAB software. Therefore, rule bases of the estimators are formed automatically with the number of inputs and number of MFs. After the ANFIS structure is constructed, learning algorithm and training parameters are chosen. backpropagation or hybrid learning can be used as a learning algorithm. The hybrid learning algorithm is used in this study. Parameters in the algorithm are epoch size (presentation of the entire data set), error tolerance, initial step size, step size decrease rate, and step size increase rate. Since there is no exact method in literature to find the optimum of these parameters a trial and error procedure is used. In all trainings, they are taken as 10, $1x10^{-5}$, 0.01, 0.9, and 1.1, respectively as default constant value as proposed in MATLAB .

MATLAB fuzzy logic toolbox is used to design ANFIS estimators' structures. Using the given training data set, the toolbox constructs an ANFIS structure using either backpropagation algorithm alone, or in combination with least squares type of method (hybrid algorithm). ANFIS model can be generated either from the command line, or through the ANFIS editor GUI. In this study, ANFIS Editor GUI is used to generate the ANFIS models with the chosen design parameters in construction phase. Written MATLAB code is used to train the ANFIS structure in the training step. This code is given the use of the ANFIS editor GUI can be found in program help files.

The steps in ANFIS estimator design in this study utilizing the MATLAB fuzzy logic toolbox are as follows:

1. Generated training data is loaded to the Editor GUI.
2. Design parameters, number of input MF, type of input and output
MF, are chosen. Thus, initial ANFIS structure is formed.
3. The code for the training is run with the initial structure.
4. ANFIS structure constituted after training is saved to use as an estimator.

V. Generation of Training Data

If the operating input-output data are outside their training data range, estimator will not operate accurately. As a result, the training data set should possess sufficient operational range including the maximum and minimum values for input-output variables. The data set should include data for each process variable, evenly distributed throughout the range for which estimation is desired.The maximum and minimum values of WIAT(^oC)(**W**eighted **A**verage **I**nlet **T**emperature) , H_2/Hc ratio and Product Separator Temperature in the catalytic naphtha reforming were determined by looking at the Test runs data of the Tehran refinery.These are considered to be their maximum changes in operation. The Range of each process variable used in training data generation is shown in Table I and testing data are shown in Table II.

TABLE I
The Range Of Process Variables

WAIT(^oC)	H_2/HC ratio	Product Separator Temp(^oC)	Ron
480	2	27	92.59
482	2.2	27	92.82
485	2.4	27	93.31
486	2.5	27.5	93.44
488	2.7	27.5	93.7
489	2.7	27.5	93.97
490	2.8	28	94.11
490	3	28	93.84
493	3	29	94.66
494	3	29	94.94
495	3.2	30	94.96
496	3.3	32	95.12
497	3.4	33	95.28
498	3.5	33.5	95.43
498	3.6	34	95.3
499	3.7	34	95.45
501.5	3.9	34.5	95.89
501.5	3.9	35	95.89
505	4	37	96.75
506	4	38	97.04
506	4	40	97.06

Thus, model simulations are done to obtain the input-output data by using these values. Then, process values and Research octane numbers are collected. In training data sets (matrix of 4 columns), first column is WAIT values second column is H_2/Hc ratio values , third column is product separator temperature values and the last is column octane number values.

TABLE II
The Range Of Process Variables

WAIT(^oC)	H_2/HC ratio	Product Separator Temp(^oC)	Ron
484	2.3	27	93.19
487	2.6	27.5	93.57
490	2.8	27.7	94.1
491	3	28	94.11
495	3.1	30	95.9
496	3.3	33	95.13
498	3.5	34	95.44
500	3.8	34	95.6
504	4	36	96.46
506	4	39	97.05

A. ANFIS estimator training

First, generated training data is loaded using the GUI Editor. Then, with chosen design parameters, initial estimator structure is constructed. For example, if three Gaussian2 MFs are used for each input and constant output MF is chosen, GUI Editor determines the initial parameters of gaussian2 MFs automatically using loaded data and constructs the initial three order 2 Gaussian MFs for each input and constant output MF ANFIS structure. Trainings of the structures are done by running the written code in MATLAB. All structures are trained in the same way.

VI. Simulation Results

After the training of the ANFIS structures, performances of estimators are investigated through the model for generalization tests.

These tests are made by utilizing the different estimator structures. The responses of the WAIT increase and increase in H_2/Hc ratio and Product Separator Temperature are obtained by simulations to verify the estimator's learning performances. In all simulations, Average testing error (ATE) scores for the error between the actual and estimated octane number are calculated as the performance criteria. Simulation results are given in Table III. Verification capabilities of the estimators can be followed considering the ATE scores giving how well these different estimator structures can generalize what they have learned. It can be seen from Figures 4 ,5 and from ATE scores that three orders 2 Gaussian MFs for each input and constant output MF ANFIS structure performance is very good.

TABLE III
Verification Test Results

Input MF	Output MF	Number of Input MF	Average testing error
Bell	constant	3	0.32
Bell	linear	3	0.23
Bell	constant	5	3.47
Bell	linear	5	2.68
Bell	constant	7	7.46
Bell	linear	7	7.68
Gaussian	constant	3	0.24

Gaussian	linear	3	0.27
Gaussian	constant	5	3.58
Gaussian	linear	5	2.48
Gaussian	constant	7	7.62
Gaussian	linear	7	7.64
Triangular	constant	3	0.25
Triangular	linear	3	0.25
Triangular	constant	5	3.42
Triangular	linear	5	1.41
Triangular	constant	7	11.03
Triangular	linear	7	10.20
Trapezium	Constant	3	0.38
Trapezium	Linear	3	0.22
Trapezium	Constant	5	5.36
Trapezium	Linear	5	5.39
Trapezium	Constant	7	18.67
Trapezium	Linear	7	16.23
Gaussian2	Constant	3	0.14
Gaussian2	Linear	3	0.16
Gaussian2	Constant	5	3.07
Gaussian2	Linear	5	1.48
Gaussian2	Constant	7	11.70
Gaussian2	Linear	7	11.57

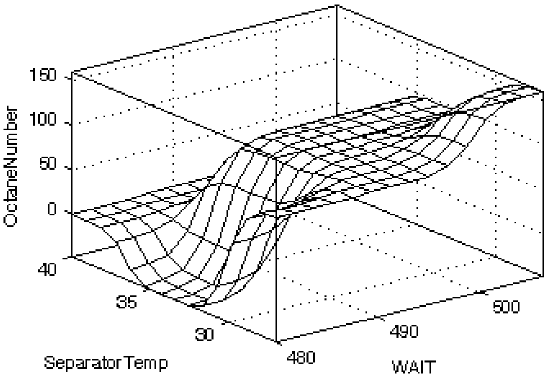

Fig. 4 ANFIS Output

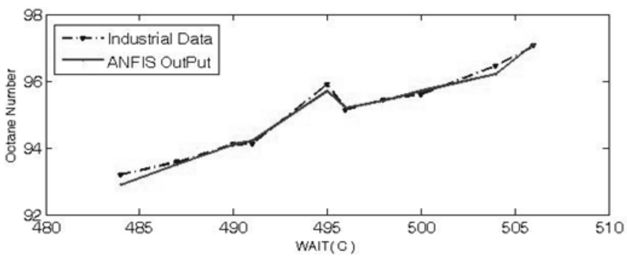

Fig. 5 Comparison of Industrial data and ANFIS output

VII. Conclusion

When investigating the generalization capabilities, it is seen from Table III that all structures give actual octane number values when the system is disturbed by process values changes. Their performances are also very good in estimating the octane number. However, it is observed that predictions of order 2 Gaussian structures are better considering the ATE scores than

That of other structures. Table III shows that minimum ATE score for Octane number is achieved from the three orders 2 Gaussian MFs for each input and constant output MF ANFIS structure.

References

[1] Guilandoust MT, Morris AJ, Tham MT. Adaptive inferential control. Proceedings of IEE Part D 1987;134(3):171–9.

[2] Montague GA, Morris AJ, Tham MT. Enhancing bioprocess operability withgeneric software sensors. Journal of Biotechnology 1992;25:183–201H.

[3] A. L. Huebner, “Tutorial: Fundamentals of Naphtha Reforming,” AIChE Spring Meeting 1999, Houston, TX, 14–18 March 1999.

[4] DAVID S. J. “STAN” JONES "Handbook of Petroleum Processing".2006 Springer

[5] Mark Lapinski, Lance Baird, and Robert James"HANDBOOK OF PETROLEUM REFINING PROCESSES" 2004 The McGraw-Hill Companies.

[6] Wang S, Jin X. Model-based optimal control of VAV air-conditioning system using genetic algorithm. Building and Environment 2000;35(6):471–87.

[7] Evren Guner."Adaptive Neuro-Fuzzy Inference Systems Applications in Chemical Processes" a Thesis Submitted to the graduate school of natural and applied Sciences the middle east Technical University