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Dedicated to Professor Liviu Literat, at his 80th anniversary

SIMULATION OF THE REACTOR-REGENERATOR-MAIN FRACTIONATOR FLUID CATALYTIC CRACKING UNIT USING ARTIFICIAL NEURAL NETWORKS

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ABSTRACT. The present work it is a successful approach for modelling the dynamic behaviour of the FCC unit, using Artificial Neural Networks (ANN). An analytical model, validated with construction and operation data, has been used to produce a comprehensive input-target set of training data. The novelty of the model consists in that besides the complex dynamics of the reactor-regenerator system, it also includes the dynamic model of the main fractionator. A new five-lump kinetic model for the riser is also included. Consequently, it is able to predict the final production rate of the main products, gasoline and diesel. The architecture and training algorithm used by the ANN are efficient and this is proved by the results obtained both on training set and set of input-target data not met during the training procedure. The same good ANN performance has been obtained by the comparison between dynamic simulations results emerged from the ANN model versus first principle modelling, both using the same randomly varying inputs. The computation time is considerably reduced when using the ANN model, compared to the use of the analytical model. The presented results show the incentives and benefits for further exploiting the ANN model as internal model for Model Predictive Control industrial implementation.

Keywords: *Fluid Catalytic Cracking Unit, Artificial Neural Networks, dynamic modelling*

INTRODUCTION

A modern petroleum refinery is composed of processing units that convert crude oil into valuable products such as gasoline, diesel, jet fuel, heating oil, fuel oil, propane, butane, and several secondary chemical feed stocks. Fluid Catalytic Cracking (FCC) is one of the most important conversion processes in a petroleum refinery, Figure 1. The main goal of this unit is to

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convert high-boiling petroleum fractions called gasoil into high octane gasoline, high cetane diesel and heating oil. The process is complex, incorporating most processes of chemical engineering fundamentals, such as fluidization, heat/mass/momentum transfer and separation by distillation.

As presented in the schematic representation of FCCU, raw material is mixed with the regenerated catalyst in the reactor-riser. The cracking reactions and coke formation occur in the riser and the important products are then separated in the main fractionator. Due to coke deposition the deactivated catalyst needs to be regenerated in the regenerator [1].

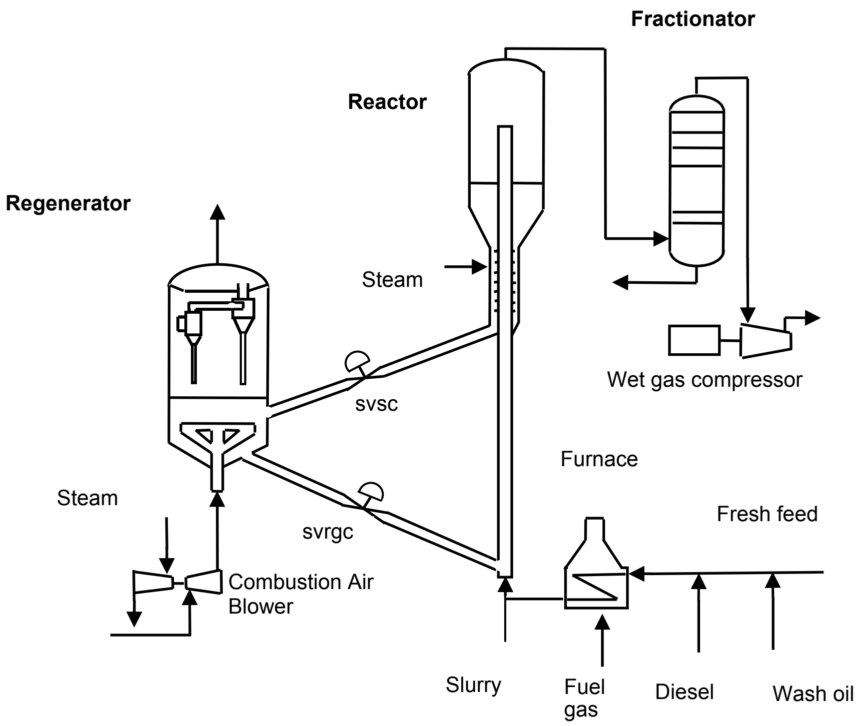

Figure 1. Schematic view of the FCCU plant.

Mathematical modelling in the chemical engineering field has a multidisciplinary character, dealing with different processes that have to be described. The mathematical models can be used in the system design, process control, identification of possible failures, training the operating personnel but also for the safety operation and assessment of environmental impact of the process.

From the point of view of the relationship between variables of a system, the models may be either analytical or statistical. Statistical mathematical models are based on observation data and measurements originating from the process (such as the Artificial Neural Networks models). Development of the analytical models is complex and time consuming as they imply a good knowledge of the phenomena and processes taking place inside the modelled system. They imply special instruction of a specialist in order to develop the specific equations. Statistical mathematical models are useful because they are simple from mathematical point of view and they do not need extended knowledge about the system, phenomena and processes underlying the system.

ANN models are able to capture the complexity of the intrinsic processes featuring the global process behaviour. Artificial Neural Networks are composed of simple elements, neurons, operating in parallel. The network function is determined by the connections between its neurons. The weighted connection paths link every two neurons to each other, the weighting structure providing the total network performance. Statistical models developed by means of ANNs and using process data are efficient alternatives to the traditional analytical models [2-4].

RESULTS AND DISCUSSION

The performance of a trained network can be measured by the errors on the training, validation and test sets, but it is often useful to investigate the network response in more detail. A regression analysis between the network response and the corresponding targets was first performed. The correlation coefficient (R-value) between the outputs and targets it is an efficient measure of how well the variation in the output is explained by the targets. For the training test the correlation coefficient, R-value, showed high values revealing a good correlation between targets and outputs.

The ANN was first designed and subsequently the quasi-Newton Levenberg-Marquardt algorithm was used to train the network. The 23 ANN-inputs are: spent and regenerated catalyst valve position; gasoline and diesel composition at the bottom and top of the main fractionator, gasoline and diesel composition on the 36^{th} and the 37^{th} stage of the main fractionator, reactor and regenerator temperature, main fractionator pressure, regenerator pressure, reactor and regenerator catalyst inventory; coke amount on the regenerated and spent catalyst; combustion air blower and wet gas compressor pressure; velocity of spent and regenerated catalyst, inventory of gas. All inputs are considered at the *t* sampling time. The last 21 variables are the process state variables and also represent the ANN outputs, but they are considered at the next sampling time, $t+\Delta t$.

A set of 201 input and output data (input/target pairs), provided by the FCCU analytical model, has been used for the ANN model development. The entire set has been divided into a set of data used for training the ANN and the rest for testing the quality of the training process.

Both for the training and testing sets of data, the R-correlation coefficient is very close to unity, indicating a very good fit between targets and the ANN model response and demonstrating a very good generalization property of the designed and trained ANN, Figure 2.

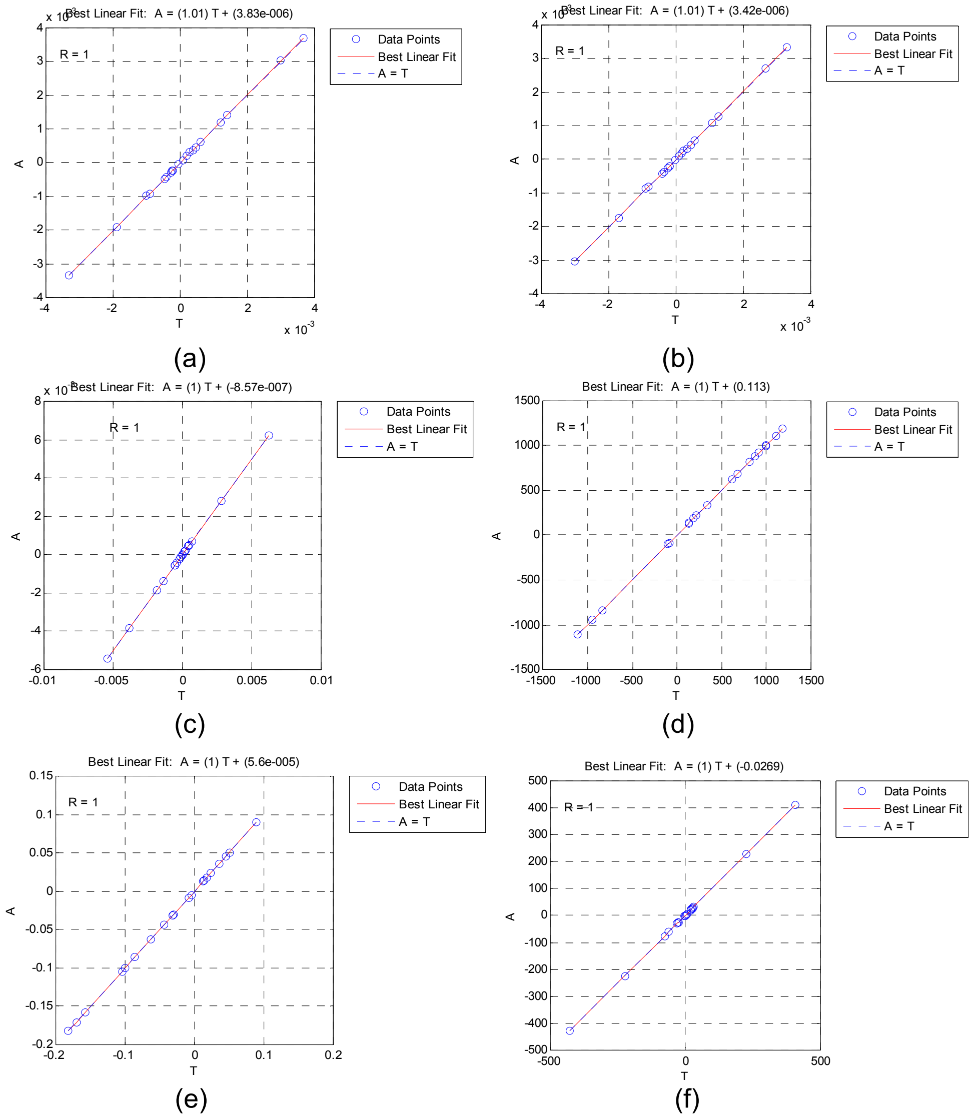

Figure 2. Results of the regression analysis between the ANN model response and the corresponding targets (testing set of data): (a)- gasoline composition on top of main fractionator, (b)- diesel composition on bottom of main fractionator, (c)- reactor temperature, (d)- column pressure, (e)-regenerator temperature, (f)- regenerator pressure.

The network outputs are plotted versus the targets as open circles. The best linear fit is indicated by a dashed line. The perfect fit line (output equal to targets) is indicated by the solid line. Figure 2 also shows that it is difficult to distinguish the best linear fit line from the perfect fit line, as they actually merge. The data set used for training has been chosen in correlation to the number of neurons in the hidden layer and covering the operating range of change of the input and output variables.

As a second, more comprehensive test, a random amplitude sequence has been generated for the input (manipulated) variables of the FCCU process: spent and regenerated catalyst slide valve opening position. They having random changes equally distributed in time. Within this final and complex test have been compared the induced evolutions of the process variables described by the ANN and the analytical models. The random amplitude sequence has been generated for both considered input (manipulated) variables with random changes equally distributed in time at multiples of 3000 seconds, as presented in Figure 3. The simulation has been performed for 15000 seconds and the evolution of the most important FCCU output variables was investigated and presented in Figure 4.

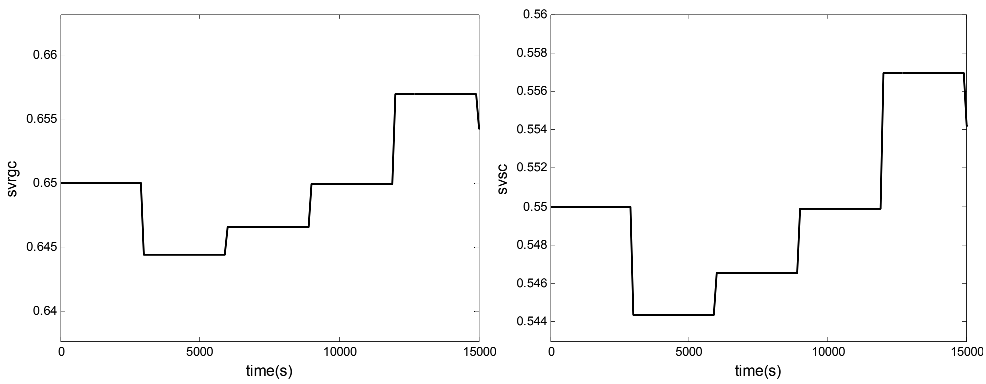

Figure 3. Amplitude sequence of the spent (svsc) and regenerated (svrgc) catalyst slide valve opening position.

The trained ANN is designed to predict one step ahead into the future the behaviour of the process variables. Applied repeatedly, the dynamic ANN predicts the time evolution of the state variables over a desired future time horizon. Again, this randomly generate testing set of data is completely different of the training one and not yet seen by the ANN.

The dynamic simulation results of the trained ANN model for the FCCU, compared to the analytical model, are shown in the Figure 4. As it may be noticed from these results, the developed ANN model has good dynamic performance. Results show the capability of the ANN model to capture the time evolution of the most important FCCU output variables.

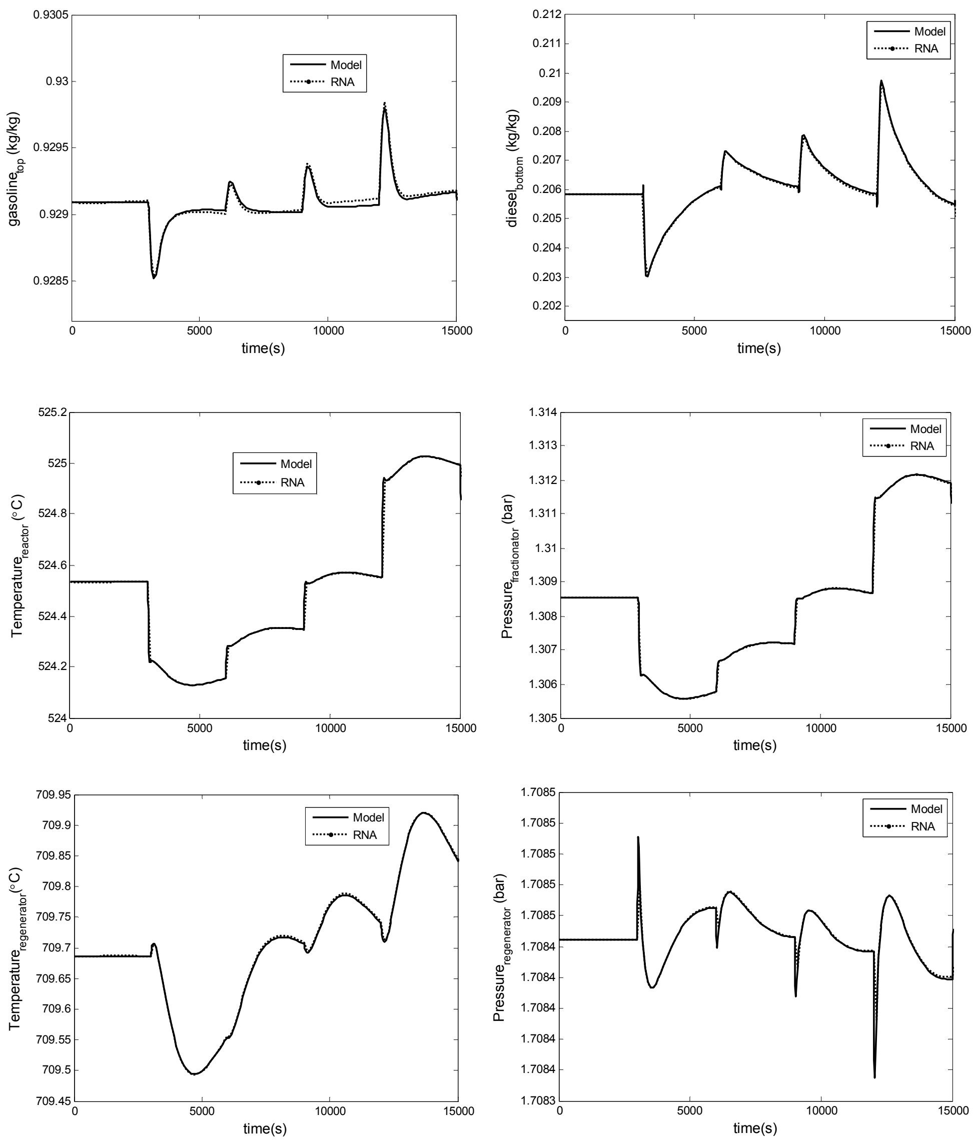

Figure 4. Comparative simulation results of the ANN and analytical model for the set of the most important FCCU variables.

It has been measured and compared the computation time needed for the dynamic simulation, using both the FCCU analytical and ANN based model. It was observed a substantial computation time saving in the case of the ANN. Using the ANN model the computational time is about 10 times shorter compared to the first principle model requirement. This computation time reduction may have an important benefit on the real time implementation of the model based control algorithms.

CONCLUSIONS

The paper presents the simulation results of successfully using Artificial Neural Networks for modelling the dynamic behaviour of the complex FCC unit. First, a comprehensive input-target set of training data were produced using the FCCU analytical model. The first principle model was previously validated with experimental data taken from a real industrial FCC unit, Rompetrol Refinery, Romania. Correlation coefficients close to unity are shown on both training and testing steps, the last one being performed on sets of input-target data not met during the training procedure. The favourable fit between results emerged from the ANN versus analytical modelling, using randomly varying inputs, showed again that the ANN architecture and training algorithm are very efficient. They demonstrate a good generalization property of the ANN. The ANN developed model substantially reduces the computation effort and supplies the potential control algorithm with speed necessary for real time implementation. Due this favourable feature, the trained ANN model for the complex FCCU can be successfully used, as inherent model, for FCCU Nonlinear Model Predictive Control. This popular advanced control strategy may be efficiently used for improving the quality and the productivity of the gasoline and diesel products.

EXPERIMENTAL SECTION

An FCCU analytical model was available and it served as a rich database needed for the ANN training and testing procedure. The FCCU model has been developed based on reference construction and operation data taken from an industrial unit: Rompetrol Refinery, Romania. The new developed complex model of the FCCU reactor-regenerator-main fractionator and auxiliary systems (wet gas compressor, air blower, feed and preheat system, catalyst circulation lines) is a high order differential-algebraic equations system, consisting in 933 differential equations and more than 100 algebraic equations. The analytical model parameters have been validated with construction and operation data from the industrial unit. The developed analytical model is able to capture the major dynamic effects that may occur in the industrial FCCU system.

The ANN architecture for the FCCU statistical model is a double-layer feed-forward one with the backpropagation training algorithm used for computing the network biases and weights [5, 6]. In the ANN architecture two layers of neurons have been considered. The input layer has 23 neurons, in the hidden layer 26 neurons have been used and the output layer consists in 21 neurons. The number of nodes in the hidden layer has been set on the basis of a trial and error process. Two ANN activation functions have been utilized: the tansing sigmoid transfer function for the hidden layer and the purelin linear transfer function for the output layer. The quasi-Newton Levenberg-Marquardt algorithm was employed for training the ANN. Overfitting has been avoided by the early stopping method which improved generalization. Random initial conditions have been used for the weights and biases, during the set of repeated sequence of training steps, in order to prevent convergence to undesired local minima. For improving the training procedure all input-output training data have been normalized using the maximum and minimum values of the input and output sets of data.

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