Review of neural network modelling of cracking process

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Abstract. Cracking process is a very important process that converts low value products into
high value products such as conversion of naphtha into ethylene and propylene. The process is
nonlinear with extensive reaction network. Thus, nonlinear technique such as artificial neural
network is explored to develop the model of the system. The paper will review and discuss the
research works done on the technique in modelling cracking process using artificial neural
network starting from early 1990s until recent development in 2015. Timeline is provided to
show progression of work done throughout the years, the main issues addressed, and the
proposed techniques for each. In the next section, the main objective of each work and each
techniques explored by previous researchers is discussed in more detail. A table that
summarizes previous works is provided to show common works done throughout the years.
Lastly, potential gap for future works in the area is highlighted.

1. Introduction
Cracking is a very important process as it has the ability to convert low value heavies material such as
heavy vacuum gas oil and atmospheric gas oil into high value ethylene and propylene. There are three
prominent methods for hydrocarbon cracking i.e. steam cracking, thermal cracking, and catalytic
cracking. Cracking process is nonlinear and semi-continuous, contributed by its extensive reaction
networks, continuous deposition of by-product, and constantly changing operating condition.
Throughout the cracking period, coke will form as by-product and deposit in the coil which lowering
the heat transfer coefficient of the coil, and composition of the feed will also start to change as the
fresh feed will be mixed with recycled feed. Due to that, operating condition at the beginning of the
process will continue to change until coke deposit layer has become so thick that the heat input
required will cause the coil metal to reach maximum tube metal temperature. By that time, operator
will stop the cracking process and initiate decoking process to remove the coke.

Looking at the nonlinear and continuously changing nature of the cracking process, researchers and
industrial practitioners in the area of system identification have started to explore non-linear
identification technique such as Artificial Neural Network (ANN), which are known to be able to
handle nonlinearities. They also incorporate multimode model to develop inferential model that can
best represent the process under different operating condition. This paper will review the previous
research work on modelling of cracking process using ANN. Finally, from all the works reviewed, the
research gaps will be highlighted for future research.

2. Progression of ANN modelling of cracking process
Modelling cracking process initially starts with developing a first principle model (FPM) from mass,
momentum, and energy balances couple with cracking reaction mechanism. The attempt to develop
FPM proved to be very extensive plus the amount of assumptions that need to be made to simplify the
reaction network and determining many other unknowns [1]. Since then, empirical techniques such as
ANN have been explored instead of FPM.
2.1. Overview of ANN research progress

ANN is one of the most attractive nonlinear techniques used by researchers for modelling the cracking process. In 1994, researchers start to explore ANN to model cracking process. The works starts with Feng et al. which used Multilayer Perceptron (MLP) with functional input to model thermal cracking furnace [2] and McGreavy et al. which used conventional MLP to model Fluid Catalytic Cracking (FCC) reactor [3]. Since then, the efforts to improve the method continue until today. As shown in Figure 1, earlier effort focused on utilizing single hidden layer feedforward network. From year 2000 onwards, contributed by more research in the area, researchers started to take notice of the limitations of ANN and focused their work on improving the techniques.

In early 2000, two important aspects of modelling have been explored – online implementation and model validity under different condition. Realizing the importance of maintaining the ANN model during actual plant operation, Nagy et al. has introduced adaptive ANN to enable online training of the model [4]. Another researcher take notice of changing operating conditions of cracking at the feed, after mixing with recycle feed, and at furnace run length that is caused by deposition of coke. In the work of Zhuang and Yu, a method using dynamic biases has been proposed to cater for the changing operating condition [5]. Normally during actual plant operation, plant dynamics consistently change due to many factors and thus, the training dataset used during offline training might not cover all operating conditions. This type of data is considered as unseen data. Bootstrap Aggregated Neural Network (BANN) has been introduced to enhance the generalization ability of the network to work with unseen data [6,7].

During the development of the model, many researchers work on improving the prediction errors of the model as well as improving the computation time. Huge amount of training data leads to long computation time and it can be difficult for online training. To reduce computation time and training load, an effort to reduce dimensionality of the data has been done by integrating Principle Component Analysis (PCA) into the network input as demonstrated in [8,9]. Starting from year 2006, researchers have started to combine ANN with other methods creating hybrid such as combination of FPM with ANN [10], incorporate Genetic Algorithm (GA) into ANN to optimize network parameters, which is known as GA-NN technique [10], and integrate Fuzzy Inference System (FIS) into the ANN layers and called as ANN-FIS model [1]. Another research work on this area is using the conventional Feedforward MLP and also Radial Basis Function NN for the modelling. The improvement proposed is more towards optimizing the cracking furnace operation parameters by using evolutionary methods such as Cultural Algorithm (CA), Differential Evolution algorithm (DEA) [11], Particle Swarm Optimization (PSO) [12,13] and GA [14,15] to vary input parameters in order to maximize output.

Within the span of 20 years, the research works have varied from exploring different structures and network configurations to improve prediction error until incorporating evolutionary methods to optimize cracking furnace operation.

2.2. Summary of research works from 1994 until 2015.

In this section, summary is provided for each paper that is related to the application of ANN in modelling cracking process, covering thermal cracking, steam cracking, and catalytic cracking. In the year 1994, Feng et al. [2] has ventured into using ANN to model thermal cracking of naptha, with addition of using functional units at input layer. A model has been developed to predict the yield of ethylene, the yield of propylene, and Kinetic severity function (KSF). McGreavy et al. has explored the use of ANN in modelling FCC to predict yield distribution of main products of light hydrocarbons and byproducts such as coke [3]. These two are the first attempt to model cracking process using ANN.

Elkamel et al. has explored the use of feed forward network to model hydrocracking unit for light vacuum gas oil [16]. A multiple inputs multiple outputs model has been used, with different model has been developed for different modes of operation, which are the Aviation Turbine Kerosene (ATK) mode and middle distillate mode. Result shows that different output has different errors produced.
Nagy et al has developed two ANN models to be used with Model Predictive Control (MPC) for FCC unit [4]. One is offline-trained and the other is adaptive. Adaptive ANN is trained online using past values of manipulated and controlled variables, to cater for unmeasured process disturbances. Both models shows superior performance compared with PI controller, and adaptive is showing better result than offline ANN. GA method is proposed to improved convergence of learning. Data used in the research is obtained from simulation through MATLAB FCCU package.

Research work by Michalopoulos et al. focused on finding the optimum structure for good generalization abilities [17]. Through trial and error, the optimum structure is obtained. The MLP model of FCC to predict percent conversion is compared with other non-linear statistical model derived from previous research. It proved to shows better performance than the statistical model. Through previous experience, it is acknowledged that cracking process exhibit changing process condition after the start of the process. Researchers start to focus on that aspect during modelling. The first attempt has been done Zhuang and Yu to explore the use of recurrent neural network and introduced dynamic biases to cater for different feed conditions and running phases of the steam cracking furnace of ethane-naphtha mixture [5]. Comparison has been made between Backpropagation (BP) and Elman network. The result shows that the use of dynamic biases significantly improves the accuracy of the model and convergence time. The proposed structure achieved convergence in lower epoch value than BP network. Another similar research by Zhu and Li model the cracking furnace using two-layer network, with the first layer function is to determine the operating condition and the second layer is a layer of BANN with sequential training specific for each operating condition [9]. Both methods avoid generalization and develop a specific method to identify the operating condition and introduce a solution for each condition.

Another research group is working on reducing computation time of network learning. In order to do that, the input data need to be reduced. Zhuang and Yu [8] have proposed a PCA in combination with dynamic neural network to model naphtha cracking furnace and predict the cracking severity. The procedure to conduct the PCA has been presented clearly in the paper for reference. Output of PCA becomes an input to the Elman network. Combination of PCA with Elman network shows better prediction than BP network and Elman network. Zhu and Li have combined PCA with Input Training Neural Network (ITNN) to develop a nonlinear PCA [9]. The output from the PCA-ITNN is input into the Radial Basis Neural Network (RBNN) to produce a model for naphtha cracking furnace to predict

**Figure 1.** Evolution of ANN modelling of cracking process

| Year | Event |
|------|-------|
| 1990 | 1994 First attempt in using ANN |
| 1995 | 1999 Use ANN to model different mode of catalytic cracking |
| 2000 | 2000 Starts to explore adaptive online-trained NN |
|      | 2003 Introduce recurrent NN with dynamic biases for different operating condition |
|      | 2004 First use of BANN to enhance generalization and attempt to combine PCA with ANN |
| 2005 | 2006 Explore the feasibility of using hybrid of ANN and 1st principle |
|      | 2007 Include PSO as part of process parameter optimization |
| 2010 | 2010 Explore the use of GA for process parameter optimization |
|      | 2011 Fuzzy inference system is integrated to cater uncertainty. |
|      | Incorporate GA in learning algorithm to improve prediction error |
| 2015 | 2013 – 2014 More application of GA and PSO as optimization tools |
ethylene and propylene yield. The integration of PCA not only increases learning speed, it also reduces prediction error primarily due to the noise removal and dimensionality reduction by PCA.

The research by Zhou et al. has introduced a new method of ANN. Two ANN models of cracking furnace is developed to predict product yields and cracking degree [6]. The first model is MLP trained by LM algorithm and the second one is using bootstrap aggregated with sequential training. However, the MLP is found to be lacking generalization abilities and prone to error when presented with unseen data. The proposed Bootstrap Aggregated Network (BANN) enables several models of ANN to be developed with different objective. Then, the outputs of individual networks are combined to give overall output and capable of producing better performance than single MLP. Zhou et al. has also utilized BANN with additional of one layer to determine process operating condition prior to proceeding to BANN layer [7]. In the work, BANN model is developed for each operating condition.

To improve the performance of ANN and overcome its limitation, several researchers have proposed hybrid technique which is a combination with first principle model, genetic algorithm, or fuzzy logic. The first one to propose is Bhutani et al. whereby three methods has been explored to model industrial hydrocracking unit [18]. The method explored are First principle model (FPM), ANN model, and a combination of both (hybrid model). The three models have been compared and evaluated, the result shows that ANN model alone provide much more robust and less absolute percent error compared to hybrid and FPM. Wang and Xu in their research developed ANN model of cracking furnace and introduces GA in the network learning algorithm to utilize its stochastic properties and improve likelihood of finding error surface global minima [10]. To handle uncertainty in the process, Sedighi et al. has introduced Fuzzy inference system into the scope and coupled it with neural network [1]. The NN-FIS has been compared with regular ANN and First principle model. Evaluation between models has been done using Analysis of Variance (ANOVA) to see prediction capability of each. NN-FIS shows superior performance of all three. The downside of NN-FIS is that it is very specific to feed type and furnace type. New models need to be developed for new feed and reactor.

In the recent years, more researchers start to focus on developing method to search for optimum process parameters in order to maximize product yields. Thus, ANN combined with evolutionary methods such as PSO, GA, CA, and DEA comes into the scene. PSO starts to be explored by Li et al. where naphtha cracking furnace has been modelled using single hidden layer network, and Multi-objective PSO has been incorporated to find the optimum operating parameter of the furnace that will maximize yield of ethylene and propylene [11]. Several other researches also using PSO, such as Geng et al., has explored the combination of Multi-modes PSO (MMPSO) and Radial Basis Function Neural Network (RBFNN) to model cracking furnace [13]. The model will be integrated with advanced process control system of COT to optimize cracking depth and maximizing ethylene and propylene yields. MMPSO has been incorporated to further optimize the ANN model.

In their work, Pu and Liu have introduced a new type of optimization algorithm. The work focuses on developing a model for monitoring process state. Elman network has been used to model cracking furnace severity state, instead of the typical product yield. The model has been integrated with Cultural algorithm (CA) and Differential Evolution algorithm (DEA) focuses on the training. The network output will be used as tool to monitor cracking severity [12].

Liu et al., in their research, has focused on the aspect of cycle oil as recycle feed to FCC after considering that cracking behavior of cycle oil is largely unknown and it affect cracking severity [14]. RBFNN has been used to develop the model to product light oil yield, and GA and PSO has been used to find optimum operating parameters to maximum yield of light oil. Bispo et al. has modelled an FCC unit using Feedforward ANN and expected to integrate the inferential model in Model Predictive Control system [15]. GA and PSO method has been used in their work to obtain optimum operating condition.
### Table 1. Summary of techniques employed in cracking process ANN modelling

| Technique employed          | Issues to be solved                  | Year                      | Reference |
|-----------------------------|--------------------------------------|---------------------------|-----------|
| MLP                         | Modelling                            | 1994, 1999, 2000, 2001, 2006, 2007, 2014 | [2] [16] [4] [17] [18] [19] [20] [11] [21] [10] [15] [3] |
| Adaptive NN                 | Changing process condition online    | 2000                      | [4]       |
| Elman NN                    | Modelling                            | 2004, 2010                | [8] [12]  |
| Radial Basis Function NN    | Modelling                            | 2006, 2010, 2013          | [9] [13] [22] [14] |
| Recurrent NN                | Modelling                            | 2003                      | [5]       |
| Bootstrap Aggregated NN     | Model generalization                 | 2004, 2006                | [6] [7]   |
| Hybrid FPM-NN               | Explore combination of method        | 2006                      | [18]      |
| Hybrid GA-NN                | Finding error global minima          | 2011                      | [10]      |
| Hybrid NN-FIS               | Uncertainty in the process           | 2013                      | [1]       |
| Optimization with GA        | Reactor optimum parameters           | 2010, 2011, 2013, 2014    | [22] [14] [15] |
| Optimization with PSO       | Reactor optimum parameters           | 2007, 2010, 2014          | [11] [13] [14] [15] |
| Optimization with CA and DEA| Reactor optimum parameters           | 2010                      | [12]      |
| Integration with PCA        | Reduce data dimensionality and computation time | 2004, 2006                | [8] [9]   |

### 3. Future Works

There are still many research gaps that can be addressed in future works. First, the gap is in the development of a complete severity control system package that consist of fault diagnosis system, data pre-processing, online ANN model training, post-processing, as well as implementing the model online in actual plant. Currently, no such work has been reported in journal. Secondly, it has been observed that different practitioners used different methods and different procedures to develop the ANN model. This has resulted in difficulties to compare the result of each work and also resulted in slow progression in the area. Thus, there is a need to establish standardized methodology and procedures that can be applied to build ANN model for different cracking process and different cracking feed. Lastly, throughout the years, it has been observed that very few works have been done to improve the learning algorithm. As highlighted in one of the works, one of the challenges of ANN is long computation time and the learning to stop at local minima in the error surface [10]. Thus, it proposed that more work needs to be done to develop a method to improve the learning speed as well as the likelihood of finding global minima.

### References

[1] Sedighi M, Keyvanloo K, and Towfighi J 2011 Modeling of thermal cracking of heavy liquid hydrocarbon- application of kinetic modeling, artificial neural network, and neuro-fuzzy models *Ind. Eng. Chem. Res.* **50** 1536–1547

[2] Feng Q, Jinshou Y, and Weisun J 1994 Modelling of industrial thermal cracking furnaces via functional-link artificial neural network *Industrial Technology. Proceedings of the IEEE*

[3] McGreavy C, Lu M L, Wang X Z and Kam E K T 1994 Characterisation of the behaviour and product distribution in fluid catalytic cracking using neural networks, *Chemical Engineering Science* **49** (24 A) 4717-4724
[4] Nagy Z, Agachi S, Bodizs L, 2000, Adaptive neural network model based nonlinear predictive control of a fluid catalytic cracking unit European Symposium on Computer Aided Process Engineering Elsevier Science B.V 10

[5] Zhuang X F, Yu J Z 2003 Modelling ethylene and propylene yield for cracking furnace based on a new kind of recurrent neural network. The Fourth International Conference On Control And Automation (ICCA '03), 10-12 June 2003, Montreal, Canada

[6] Zhou Q, Zhang J, Xu Y 2004 Predicting product yield profile and cracking degree in ethylene furnace 8th International Conference on Control, Automation, Robotics and Vision, Kunming, China. 6-9th December 2004

[7] Zhou Q, Xiong Z, Zhang J, and Xu Y 2006 Hierarchical neural network based on product quality prediction of industrial ethylene process Springer-Verlag Berlin Heidelberg

[8] Zhuang X F and Yu J S 2004 A novel approach for modelling cracking furnace severity, Proceedings of the 5th World Congress on Intelligent Control and Automation, June 15-19, 2004

[9] Zhu Q X and Li C F 2006 Dimensionality reduction with input training neural network and its application in chemical process modelling Chinese J. Chem. Eng. 14(5) 597-603.

[10] Wang J F, Xu H Y 2013 Ethylene plant genetic network modelling and optimization IEEE.

[11] Li C F, Zhu Q X and Geng Z Q 2007 Multi-objective particle swarm optimization hybrid algorithm with neural network: An application on industrial cracking furnace, Ind. Eng. Chem. Res. 46 3602-3609

[12] Yunxia Pu Y X and Liu M D 2010 Early warning technology of cracking severity based on improved cultural differential algorithm, Proceedings of the 8th World Congress on Intelligent Control and Automation, July 6-9 2010, Jinan, China

[13] Geng Z Q, Shang T F, Li F 2010 Integrated MMPSO and RBFNN for optimal control of cracking depth in ethylene cracking furnace 2010 Sixth International Conference on Natural Computation (ICNC 2010)

[14] Liu Y B, Tu Y S, Li C Y, Yang C. H. 2013 Catalytic cracking and PSO-RBF neural network model of FCC cycle oil China P. E. T. Process P. E. 15 (4) 63-69

[15] Bispo V D S, Silva E S R L, Meleiro L A C 2014 Modelling, Optimization, and control of a FCC unit using neural networks and evolutionary method, Engevista, 16 (1) 70-90

[16] Elkamel A, Al-Ajmi A and Fahim M 1999 Modelling hydrocracking process using artificial neural network Petrol. Sci. Technol. 17 (9&10) 931-954

[17] Michalopoulos J, Papadokonstadakis S, Arampatzis G and Lygeros A 2001 Modelling of an industrial fluid catalytic cracking unit using neural networks Trans IChemE 79 (A) March 2001

[18] Bhutani N, Rangiaah G P and Ray A K 2006 First principles, data-based, and hybrid modelling and optimization of an industrial hydrocracking unit Ind. Eng. Chem. Res., 45 7807-7816

[19] Eckert E, Belohlav Z, Vanek T, Zamostny P, Herink T, 2007 ANN modelling of pyrolysis utilizing the characterisation of atmospheric gas oil based on incomplete data Chem. Eng. Sci. 62 5021-5025

[20] Nabavi R, Niaei A, Salari D, Towfighi J 2007 Modelling thermal cracking of LPG - Application of artificial neural network in prediction of main product yield J. Anal. Appl. Pyrol. 80 175–181

[21] Niaei A, Towfighi J, Khataee A R, Rostamizadeh K. 2007 The use of ANN and mathematical model for prediction of the main product yield in the thermal cracking of naphtha Petrol. Sci. Technol. 25 967-981

[22] Shang T F, Geng Z Q 2010 Online operation optimization based on GA-RBF network in ethylene cracking furnace 978-1-4244-7330-4/10 IEEE