NEURAL NETWORK BASED INFERENTIAL MODEL FOR ETHANE STEAM CRACKING FURNACE

by

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Mohd Nazarudin Bin Rosli

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LIST OF ABBREVIATIONS

AFR	Air-fuel ratio
ANN	Artificial neural network
ANOVA	Analysis of variance
APRBS	Variable amplitude pseudo-random binary signal
ART	Adaptive resonance theory
BANN	Bootstrap aggregated neural network
BP	Back propagation
BR	Bayesian regularization
CIP	Coil inlet pressure
COP	Coil outlet pressure
COT	Coil outlet temperature
DV	Disturbance variable
EER	Ethylene-ethane ratio
ELM	Extreme learning machine
FCC	Fluid catalytic cracking
FFNN	Feedforward neural network
FIS	Fuzzy inference system
FPM	First principle model
GA	Genetic algorithm
GRNN	General regression neural network
ITNN	Input-training neural network
KSF	Kinetic severity factor
LM	Levernberg-Marquardt

MIMO	Multiple Input Multiple Output
MISO	Multiple Input Single Output
MLP	Multilayer Perceptron
MPC	Model predictive control
MTM	Maximum tube metal temperature
MV	Manipulated variable
PCA	Principle component analysis
PDF	Probability density function
PER	Propylene-ethylene ratio
PRBS	Pseudo-random binary signal
PSO	Particle swarm optimization
RBF	Radial basis function
RMSE	Root mean squared error
TMT	Tube metal temperature
SCG	Scale conjugate gradient
SHC	Steam-hydrocarbon ratio
SOM	Self-organizing map
SS_ethane	Steady state/nominal ethane flow rate
SS_ethylene	Steady state/nominal ethylene flow rate

MODEL PENGANGGARAN BERDASARKAN RANGKAIAN NEURAL BAGI RELAU PEMECAHAN STIM UNTUK ETHANA

ABSTRAK

Taburan hasil produk dari pemecahan ethana ditentukan melalui persampelan makmal dan alat penganalisis unsur untuk mengukur tahap pemecahan. Disebabkan alat penganalisis unsur mengambil masa untuk menghasilkan keputusan, hanya bergantung kepada alat penganalisis dan analisis makmal untuk menentukan hasil produk utama akan melambatkan tindakan kawalan segera kepada proses. Untuk menyelesaikan masalah ini, penderia penganggaran diperlukan. Dalam kajian ini, model penganggaran berdasarkan rangkaian neural telah dibangunkan

Proses pemecahan steam etana telah dimodelkan menggunakan ASPEN Plus dan disahkan dengan data industri yang diambil dari kepustakaan. Ralat relatif untuk keluaran model tersebut adalah kurang dari 10%. Model ASPEN Plus tersebut digunakan untuk pemilihan input, penilaian tidak-linear, dan penjanaan data untuk permodelan rangkaian neural. Pemilihan input menunjukkan yang lima pembolehubah memberi kesan yang penting kepada pengeluaran ethana dan etilina. Lima pembolehubah tersebut adalah tekanan reaktor, suhu keluaran reaktor, nisbah wap dan hidrokarbon, komposisi bahan masuk, dan komposisi bahan bakar. Penilaian ciri-ciri tidak linear proses tersebut menunjukkan yang proses itu mempunyai tidak balas yang tidak simetri dan mempunyai ciri-ciri kepelbagaian input. Oleh itu, proses ini boleh dikategorikan sebagai proses yang tidak linear.

Data yang dijana dari model ASPEN Plus digunakan untuk latihan, pengesahan, dan ujian. Dua kaedah telah digunakan untuk menghasilkan data tersebut iaitu secara

berturutan dan secara serentak. Empat pembolehubah diuji secara berturutan dan digabungkan menjadi profil berturutan. Data itu dibahagikan kepada bahagian untuk latihan dan pengesahan, dan data yang dihasilkan serentak digunakan untuk ujian.

Tiga model rangkaian neural, iaitu Rangkaian Neural Suap-depan (FFNN), Rangkaian Neural Regresi Teritlak (GRNN), dan Rangkaian Neural Mesin Pembelajaran Ekstrim (ELM-NN), telah dibangunkan dan dinilai melalui ketepatan ramalan dan masa pengiraan. Keputusan penilaian menunjukkan yang ketepatan ramalan ELM-NN adalah lebih tinggi dari FFNN dan GRNN. Untuk latihan pula, model terbaik untuk ELM-NN, GRNN, dan FFNN memerlukan masa 0.0068 saat, 0.35 saat, dan 12 saat setiap satu. Dari segi masa pengiraan untuk sampel data yang terbaru, ketiga-tiga model memerlukan kurang dari 0.05 saat untuk mengira satu sampel data. Walaupun begitu, masa pengiraan untuk model GRNN yang telah dilatih meningkat secara eksponen dengan peningkatan jumlah sampel data manakala model FFNN dan model ELM-NN yang dilatih tidak menunjukkan peningkatan masa pengiraan yang ketara,

Dari tiga model ini, ELM-NN memberi prestasi terbaik dari segi ketepatan ramalan dan masa pengiraan. Nilai R^2 untuk model ELM-NN adalah 91.3% dan 82.6% untuk ethana dan etilina setiap satu. Model tersebut memerlukan 0.0068 saat untuk latihan dan juga 0.0001 saat untuk mengira hasil ethana dan etilina dari data input yang baru. Ini membuatkan model tersebut sesuai untuk digunakan dalam aplikasi system kawalan penganggaran masa nyata.

NEURAL NETWORK BASED INFERENTIAL MODEL FOR ETHANE STEAM CRACKING FURNACE

ABSTRACT

The product yield distribution of ethane steam cracking is typically obtained using analysers and lab sampling. Since both methods take time to produce results, primarily depending on them to determine main product yield will hinder immediate control action on the process. In order to resolve this issue, an inferential sensor is required. In this study, a neural network based inferential model is developed.

The ethane steam cracking process has been modelled using ASPEN Plus and validated with industrial data taken from literature. The relative error (RE) of the model outputs obtained are less than 10%. The ASPEN Plus model is used for input variable selection, nonlinearity assessment, and data generation for neural network modelling. The input variable selection study found that five variables are significantly influential to the ethane and ethylene yields, namely reactor pressure, coil outlet temperature, steam-hydrocarbon ratio, feed composition, and fuel composition. Nonlinearity assessment of the process shows that the process exhibit asymmetrical response and input multiplicities characteristics, and thus, can be classified as a nonlinear process.

Data generated from the ASPEN Plus model is used for training, validation, and testing. Two methods have been used to generate the data which are sequential excitation and simultaneous excitation. Four variables are individually excited and combined to make a sequential excitation profile. Data from sequential excitation is

divided into training and validation while data from simultaneous excitation is used solely for testing.

Three neural network model, namely the Feedforward Neural Network (FFNN), the Generalized Regression Neural Network (GRNN), and the Extreme Learning Machine Neural Network (ELM-NN) are developed and they are evaluated in terms of prediction accuracy and computational time. The evaluation results show that ELM-NN prediction accuracy is higher than FFNN and GRNN. To train, the best model for ELM-NN, GRNN, and FFNN models require 0.0068 seconds, 0.35 seconds, and 12 seconds respectively. In terms of computation time of new set of input data sample, all three models require less than 0.05 seconds to compute one sample of data. However, computation time of the trained GRNN model increases exponentially with the increasing amount of data samples in a batch while for trained FFNN and trained ELM-NN model, the increment is not significant.

Out of the three models, the ELM-NN gives the best performance in terms of prediction accuracy and computational time. The R^2 of the ELM-NN model is 91.3% and 82.6% for ethane and ethylene yield respectively. The model requires 0.0068 seconds to train and 0.0001 seconds to compute ethane yield and ethylene yields from a new set of input data. This makes the model suitable for applications in real time inferential control system.

CHAPTER ONE

INTRODUCTION

1.1 Research background

Olefin is one of the most valuable products of the petrochemical industry. It is used as a feedstock in many petrochemical processes and serves as the building block for other value added products. The two most sought olefins are ethylene and propylene, with ethylene being in larger demand of the two. Among the derivatives of ethylene are polyethylene and ethylene oxide (Liu et al., 2010). Olefin is produced through a process called cracking, which in principle, converts long chains of hydrocarbons into lighter components.

1.1.1 Steam cracking process

Cracking is a very important process as it has the ability to convert low value heavies such as heavy vacuum gas oil and atmospheric gas oil into high value ethylene and propylene. There are various commercial cracking processes, namely steam cracking, hydrocracking, and catalytic cracking. For ethane feedstock, steam cracking is the prominent process to convert ethane into higher value ethylene. A typical ethylene plant process schematic is shown in Figure 1.1. Fresh ethane is mixed with superheated steam, preheated upon entering the furnace before being supplied with extreme heat in the furnace to initiate the cracking reaction. The reaction is endothermic, and will continue in the cracking coil as long as it receives heat input along the furnace. Monitoring the reaction temperature is done at the coil outlet, which is called the Coil Outlet Temperature (COT). Upon exiting the radiant section, the mixture will undergo rapid quenching in the transfer line exchanger (TLE) to stop the cracking reaction by reducing the temperature. Then, the cracked gas composition is analysed at the TLE outlet by an online analyser and a laboratory test. This is the end of the section called the Hot Section. The main products are recovered via a series of compressions, refrigeration, and distillation systems. This section is called the Cold Section. Unreacted feed together with certain products are recycled back into the furnace to mix with the fresh feed.

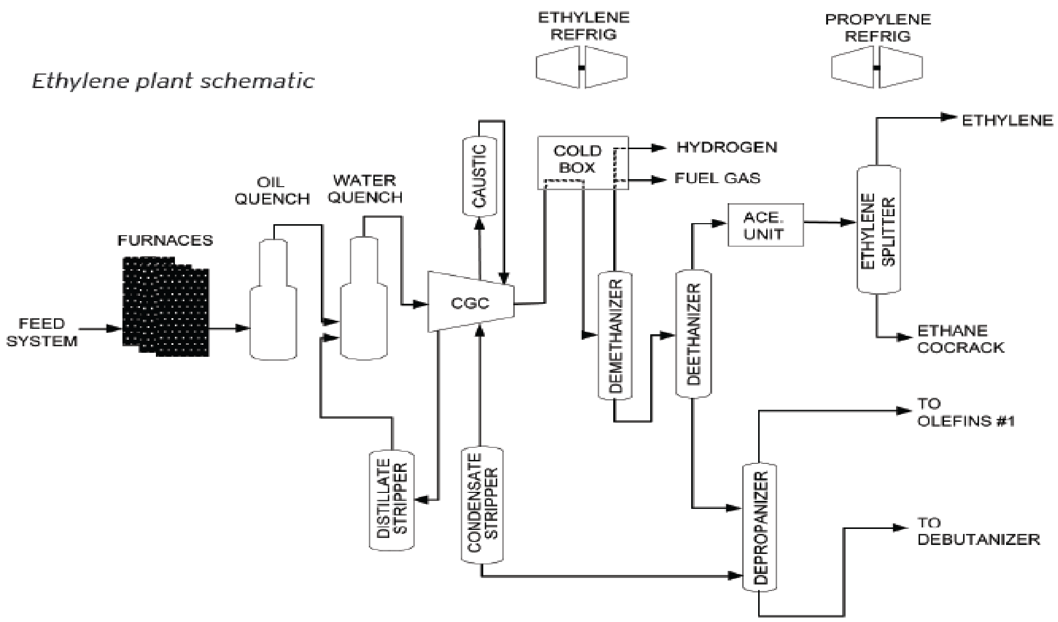

Figure 1.1: Process schematic of ethylene production plant (Samad and Annaswamy, 2011)

Throughout the run length of the furnace, the dynamics of the process slowly change as the feed composition changes after fresh feed is mixed with recycled feeds (Zhuang and Yu, 2003), and coke is deposited along the reactor tubes. The presence of the coke layer reduces the overall heat transfer coefficient of the coil and increases the heat input requirement to the reactor (Masoumi et al., 2006a, Karimzadeh et al., 2009). After a period of time, the coke deposition is thick enough to cause the heat input to the coil to be too high, making the coil temperature reach its mechanical limit, known as the Maximum Tube Metal (MTM) temperature. The furnace operation is stopped and undergone a process called decoking to remove all the coke deposits in the coils (Zhang et al., 2009). Upon completion of decoking, the furnace is started up again with fresh feed.

The depth of the cracking reactions is called cracking severity - which is dependent on feed conversion, feed composition, product composition, reactor temperature, reactor pressure, and residence time. Monitoring the severity enables plant operators to evaluate the condition of the cracking process and allows them to optimize the cracking furnace accordingly. If the severity is allowed to be too high, it leads to over-cracking, which promotes the progression of secondary reactions and the production of by-products. If the severity is allowed to be too low, it causes the under-cracking of the feedstock, producing an insufficient rate of the desired products and subsequently severing the economics of the plant. Thus, maintaining cracking severity continuously at target is paramount to ensure an optimum cracking process (Ghashghaee and Karimzadeh, 2011).

Based on the review of severity measures by Van Camp et al. (1985), the easiest method to analyse severity is by using the properties of the reactor effluent. Based on the effluent properties, two methods can be used to measure cracking severity. The first method is using a temperature-based index. Typically COT is chosen as the temperature-based severity measure due to its proportional relation to the feed conversion (Van Camp et al., 1985). The other method is by relating the severity index directly to product compositions such as Methane yield (Y_{meth}), Propylene/Ethylene ratio (PER) and Ethylene/Ethane ratio (EER) (Van Geem et al., 2005). There are pros and cons in using each severity index. While COT is the easiest to measure and control, it does not provide an accurate description of the product distribution (Van Camp et al., 1985). Changes to the process parameters will change the distribution of the product yield even though COT is continuously maintained at target. Because of that, the furnace is not operating at optimum performance (Ghashghaee and Karimzadeh, 2011). Since it is not able to accurately relate to product yield distribution, COT is not a good measure of severity.

Using a of composition-based severity index is the most informative way of measuring severity as it enables plant operators to gauge the effect of process parameters on product distributions. Setting the composition-based severity index as the control objective allows the reactor to be operated optimally in terms of production and cost, as demonstrated by Ghashghaee and Karimzadeh (2011) in their severity optimization study. Using the composition-based severity index as the control objective will also allow process adjustments towards maximum desirable products (Ghashghaee and Karimzadeh, 2011). Thus, a composition-based severity index is a better measure. In order to direct the ethane cracking severity index towards ethylene selectivity, the use of the Ethylene/Ethane ratio (EER) is proposed (Van Geem et al., 2005).

1.1.2 The need for soft sensor

The drawback of using a composition-based severity index is the dependency on the measurements from the analyser. The analyser data is infrequent and has a long sampling time, which could be up to 35 minutes per sample (Masoumi et al., 2006a). Obtaining real time product composition data that enables immediate control adjustment is not possible. One of the proposed methods to tackle this issue is by using a soft sensor (Masoumi et al., 2006a). The soft sensor is an inferential model capable of inferring the product composition of the process from secondary measurements such as temperature, pressure, and flow rate. Since the response time of the soft sensor is much faster than the analyser, it can be used as a replacement for the analyser in the process monitoring system and the severity control system.

Many chemical processes are inherently nonlinear. Some processes exhibit stronger nonlinearity compared to others (Pearson, 2006). The steam cracking process is one of the processes that exhibit nonlinearity characteristics primarily due to the interaction between process parameters, the interaction between the process equipment (Fluegel et al., 1997), and the inherent nonlinearities that come from the cracking reaction system (Xu et al., 2011). In order to accurately model the steam cracking process, the first principle method (FPM) and nonlinear empirical methods are among the suitable methods to be used. The FPM suffers from complex development processes and high computational requirements to solve the set of differential equations present in the model (Bhutani et al., 2006). In order to reduce the computational requirements, many assumptions need to be made to simplify the physics and chemistry of the system. This greatly reduces the accuracy of the model and reduces its merit. The alternative for the FPM is the empirical model, which is built from actual operating data. One of the data-based modelling method which works well with the nonlinear system is the Artificial Neural Network (ANN) (Jin et al., 2016).

1.2 Problem Statement

The ethane cracking furnace is usually operated by controlling the coil outlet temperature (COT). However, apart from temperature, the cracking severity is also influenced by other factors. Maintaining COT at target does not take into account the effect of other influencing process parameters towards the product yield. The use of the Ethylene/Ethane ratio (EER) as a severity index is a more accurate measure. Information on the actual product yield will enable adjustment of the process the parameters to maintain EER at target. However, due to the long sampling time, using the analyser data as feedback will make immediate control action not possible (Masoumi et al., 2006b). Thus, there is a need to develop an inferential model that can predict product composition based on the current operating condition. The predicted product yields will be used as the input to the severity controller until the analyser result is available (D'Hulster et al., 1980). Thus, this enables a quick response when deviation is detected in product quality.

Among the methods that can be used to develop the inferential model is the Artificial Neural Network (ANN). This method is gaining attention due to its ability to learn from available data and its capability to model nonlinear systems. Since the cracking process is known to be nonlinear (Xu et al., 2011), the ANN is suitable to be used. Apart from nonlinearity, another characteristic of the cracking process is time-variance. This is due to the changing process dynamic over time (Zhang et al., 2009). The same values of the process parameters will not produce the same product yield distribution several days later. In addition, the steam cracking furnace is never operated in full steady state condition (Ghashghaee and Karimzadeh, 2011). Thus, the inferential model has to be able to track the changing process condition (Slišković et al., 2013) and be able to update the model parameters (Iliyas et al., 2013), if necessary. In order to solve this issue, the ANN with a fast training capability is required. Among the techniques that are capable of fast trainings are the Generalized Regression Neural Network (GRNN) and the use of the Extreme Learning Machine (ELM) algorithm to train the Feedforward Neural Network (ELM-NN). Thus, the GRNN or the ELM-NN is used to develop the inferential model.