NEURO FUZZY KINETIC MODELING OF PROPYLENE POLYMERIZATION

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To my beloved parents, thank you for always being there for me, supporting me and encouraging me to be the best that I can be.

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ABSTRACT

In the present study, a neuro fuzzy kinetic model was developed to predict production rate for bulk homo-polymerization of propylene in an industrial loop reactors. The adaptive-network-based fuzzy inference system (ANFIS) technique was trained with recorded data and generated the membership function and rules which most excellent expounded the input/output correlations in the process. Three adaptive network- based fuzzy inference systems were presented. The three neuro fuzzy systems are ANFIS based grid partitioning, ANFIS based subtractive clustering, and ANFIS based Fuzzy C-means clustering. For implementation of the resent technique the MATLAB (2010a) codes were efficiently employed. The effect of different parameters for training the model was studied and the performances of consequential FIS were compared. A real-world homo-polymerization production rate data set was gathered from a typical petrochemical complex and after pre-treating was used for training of ANFIS. ANFIS model was generated and tested using training and testing data from that data set. The performance of best obtained network was checked by its generalization ability in predicting 30% of the unseen data. Excellent prediction with Root Mean Square Error (RMSE) of 0.0096 was observed. ANFIS based subtractive clustering outperformed ANFIS based grid partitioning and ANFIS based Fuzzy C-means clustering due to its fitness in the target problem. At the next step, the result of best ANFIS model was compared with a first principal model and then this model was modified and its result was also compared with ANFIS model. This paper shows the appropriateness and superiority

of ANFIS for the quantitative modeling of production rate than first principal modeling.

ABSTRAK

Dalam kajian ini, model kinetika neuro fuzzy dibangunkan untuk meramalkan tingkat pengeluaran massa-pempolimeran Homo propylene dalam sebuah reaktor loop industri. Sistem inferensi adaptif-rangkaian-berasaskan Fuzzy (anfis) teknik dilatih dengan data direkodkan dan dihasilkan fungsi keahlian dan Peraturan yang paling baik diterangkan korelasi input / output dalam proses. Tiga adaptif berasaskan rangkaian sistem inferensi fuzzy disajikan. Ketiga sistem neuro fuzzy adalah partisi grid yang didasarkan anfis, anfis berasaskan algoritma subtraktif, dan anfis berasaskan Fuzzy C-means. Untuk pelaksanaan membenci teknik MATLAB (2010a) kod yang cekap digunakan. Pengaruh parameter yang berbeza untuk latihan model dipelajari dan prestasi FIS atas sebab dibandingkan. Sebuah dunia nyata homo-pempolimeran laju pengeluaran kumpulan data yang dikumpulkan dari kompleks petrokimia yang khas dan selepas pra-mengubati digunakan untuk latihan anfis. Model anfis dihasilkan dan diuji menggunakan data latihan dan ujian dari kumpulan data. Prestasi rangkaian terbaik yang diperolehi diperiksa dengan kemampuan generalisasi dalam memprediksi 30% dari data yang tak terlihat. Excellent ramalan dengan Root Mean Square Error (RMSE) sebanyak 0,0096 diamati. Clustering berasaskan anfis subtraktif mengungguli partisi grid yang didasarkan anfis dan anfis berasaskan Fuzzy C-means kerana kecergasan dalam masalah target. Pada langkah berikutnya, hasil model anfis terbaik berbanding dengan model pokok terlebih dahulu dan kemudian model ini telah diubahsuai dan hasilnya juga dibandingkan dengan model anfis. Makalah ini menunjukkan kesesuaian dan keunggulan anfis untuk pemodelan kuantitatif tahap pengeluaran dari model utama pertama.

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INTRODUCTION

1.1 Background of Study

Polypropylene is a thermoplastic polymer, prepared by the chemical manufacturing and used in an extensive variety of applications. Loop reactors are widely used in large-scale polymerization industries because they offers low capital and maintenance cost, high production rate, high heat removal, and maintain homogeneous temperature, pressure and catalyst distribution. In this study a typical petrochemical complex was considered which its main products are olefins and polyolefins (polyethylene and polypropylene). Homo-polymer (HOMO), random-copolymer (RACO) and Impact-copolymer (IMCO) are three types of marketable PP in this complex. HOMO and RACO are produced in a loop reactor and IMCO is produced in the fluidized bed reactor. Product quality PP resins are differentiated depending on their end-use properties such as xylene soluble (XS), melt flow index (MFI), ethylene content, additive content, particle size distribution (PSD), and other physical properties such as, impact strength, hardness, flexural modulus etc.

Since Polypropylene has various types of requisitions, process upgrading is very essential in ensuring good quail ty and decreasing the producing of off spec product. Commonly, the product quality value is experimentally checked once every 4 hours later than the sample was taken from sampling point. In this occasion, the time delay to identify off spec product will lead to losses. On the other hand, Production wastage may happen during the process.

During the launch of polymerization reactors and during polymer grade transition, production rate is maintained as low as possible to minimize the production of off-spec polymer resins. Unfortunately, there is no online measurement for polymer production rate at present. In this company, it is calculated by the empirical models that are integrated into the plant distributed control system (DCS) panel. Model can be build either on the basis of mass or energy balances. Both models are acceptable agreements between themselves. Continuous online measurement data as inputs is inserted into the empirical model to obtain desired output. But, the empirical model is not able to represent the dynamic manners of propylene polymerization inside the loop reactors.

There have been relatively only some publications in relation to modeling loop reactors for olefin polymerization. Uvarov and Tsevetkova (1974), Lepski and Inkov (1977), and Ferrero and Chiovetta (1990), have modeled loop reactors as a CSTR. Zacca and Ray (1993), modeled loop reactors as two tubular divisions interrelated by completely mixed inlet and outlet zones. A comprehensive kinetic scheme that was able to deal with multisite (up to four active site types) and copolymerization (up to three monomers, one of them a diene) kinetics was presented. Reginato, Zacca, and Secchi (2003), modeled the loop reactors as a lump parameter system of non ideal CSTRs. Lately, Zamry (2009)developed a dynamic model for liquid phase propylene homo-polymerization. Although the process model had been developed in dynamic form in his study, the model estimation (carried out using the steady-state values) was not good because of error in the production rate (overall percent deviation was around 10%).

All in all, these first principal models could not overcome the complexity of reactions in polymerization process and predict output of the model with high accuracy, because polymerization happens via a diverse of reaction mechanisms that differ in complexity due to functional groups present in reacting compounds. As a substitute, a model can be build with a computer-aided system to overcome this difficulty.

1.2 Problem Statement

Polymerization reaction engineering is a extremely fascinating area of research and investigation for a lot of grounds. First, polymerization processes differ from other chemical processes cause of the dealing with the synthesis of macromolecules. Macromolecules of extremely different chain lengths are produced in polymerization reactions and the resulting molecular mass distribution plays a basic role for the determination of the end-use properties of the polymer produced. Next, a number of kinetic mechanisms are accessible for the synthesis of the macromolecules and the same monomer may manufacture dissimilar polymers depending on the chosen reaction mechanism. Third, in a number of processes very small quantities, parts per million, of impurities, may compromise catalysts performance even at plant site. Fourth, the reactor non linear behavior may be an important issue in a lot of processes and should not be neglected during reactor design. And finally, engineers of polymerization process have to cope regularly with operational complexities associated with dramatic changes in the viscosity of liquid-phase reactions, require to remove high quantities of heat released by reaction and the challenge to keep mixing patterns close to the preferred ones (Melo et al., 2003).

Moreover, having an appropriate and well-built kinetic model for a polymerization plant is a necessity because it is needed to optimize production rate and product quality while minimizing operational expenses. As a result of the reasons pointed before, polymerization reaction engineering has always been a very dynamic field and modeling of polymerization process is not straightforward.

Although there are a number of process models available in the literatures that are capable to describe the behavior of loop reactors and also predict the production rate of polymer resins, the existing models are very limited and unique to the process being studied. Usually there are several key elements in the process model that make it unique to the specific polymerization reactor. In addition, there are some assumptions in these models for simplifying, for example constant feed flow- rate, single site mechanism, and ideal mixing behavior, which introduces some errors into prediction ability of the model. For generating a new model to estimate production rate correctly, with avoiding the inaccuracy and uncertainty in the kinetic model, it is quiet important to introduced most important factors ,without any simplification, that are dealing with polymerization process into the desired model.

1.3 Objective

The objective of this study is to develop a neuro fuzzy kinetic model for bulk Homo-Polymerization of Propylene in industrial loop reactors. The model should be able to predict the polymer production rate.

1.4 Scope of Study

In realm cases, the polypropylene plant consists of many unit operations such as pre-contacting pot, in-line mixer, and baby-loop before the polymer being sent to the loop reactor. The boundary and scope of the study has been carried out as following:

i. Choice of inputs is in the black box boundary which has covered up from the baby loop until the discharge of second loop reactor. Production rate is examined as output variable.
ii. Development of a neuro fuzzy kinetic model to predict production rate of polymer for liquid phase propylene homo polymerization in industrial loop reactor at a typical petrochemical complex. The complete process model is programmed and simulated in MATLAB R2010a.
iii. Training and validation of neuro fuzzy model by using industrial data. From the industrial data file, seventy and thirty percent of all data observations were selected for training the model and estimating the generalization ability of the model, respectively.
iv. Simulation of the process to investigate plant operation. Profiles of polymer production rate is studied and compared with industrial practices.
v. Analysis on model sensitivity towards changes in process input variables, like feed concentration of catalyst active sites, and feed flow rate of hydrogen and propylene. The analysis is carried out by using two methods.

1.5 Contribution of Study

As the study is carried out based on collaboration between academia and industry, the output of study is aimed to benefit both parties. Contribution of study is described as below:

i. The developed, programmed and simulated neuro fuzzy kinetic model provides a more accurate and precise outcome to predict production rate than a first principle model in bulk propylene polymerization.

ii. Since the process is a quiet nonlinear process, neuro fuzzy modeling brings advantages because the capability to capture the nonlinear relationship between output and input elements for industry application. Forecast production rate with high accuracy will bring the company in the competitive way, when optimization is intended or troubleshooting is needed.

iii. The neuro fuzzy model is able to predict the polymer production rate, thus for the purpose of operator training, plant monitoring and troubleshooting, could be very valuable.

iv. With the presence of a reliable and robust process model, new polymerization recipes can be simulated easily, saving much time as compared to pilot-scale trial. In fact, new polymerization recipes can be formulated efficiently by having a robust model with a proper optimization procedure.