Hybrid Artificial Neural Network−Genetic Algorithm Technique for Modeling and Optimization of Plasma Reactor

Istadi*,† and N. A. S. Amin‡

Chemical Reaction Engineering and Catalysis (CREC) Group, Department of Chemical Engineering, Diponegoro University, Jln. Prof. Sudharto, Semarang, Indonesia 50239, and Faculty of Chemical and Natural Resources Engineering, Universiti Teknologi Malaysia, 81310 UTM Skudai, Johor, Malaysia

A hybrid artificial neural network−genetic algorithm (ANN−GA) numerical technique was successfully developed to model, to simulate, and to optimize a dielectric barrier discharge (DBD) plasma reactor without catalyst and heating. Effects of CH_4/CO_2 feed ratio, total feed flow rate, and discharge voltage on the performance of noncatalytic DBD plasma reactor were studied by an ANN-based simulation with a good fitting. From the multiobjectives optimization, the Pareto optimal solutions and corresponding optimal process parameter ranges resulted for the noncatalytic DBD plasma reactor owing to the optimization of three cases, i.e., CH_4 conversion and C_{2+} selectivity, CH_4 conversion and C_{2+} yield, and CH_4 conversion and H_2 selectivity.

1. Introduction

It is very promising to utilize methane and carbon dioxide in natural gas as raw materials for the production of highly valuable chemicals and clean fuels. A major difficulty for such direct methane conversion is to activate the stable C−H bonds in methane molecules using conventional catalysis. Methane conversion in the presence of oxidants, such as oxygen, is thermodynamically favored for the production of CO_x. It is very important to improve the conventional catalysts and, at the same time, to exploit other potential techniques for methane conversion. Because of high-energy electrons of the plasma reactor, it is expected that methane and carbon dioxide gases could be activated easily in the plasma environment and converted into synthesis gases and higher hydrocarbons. It is expected that a nonconventional dielectric barrier discharge (DBD) plasma reactor is an efficient tool for converting CH_4 and CO_2, greenhouse gas contributors, to synthesis gas and higher hydrocarbons at low temperature and ambient pressure.[1−5]

Numerical modeling and simulation on plasma reactors are essential for resolving the difficulties met in the measurements in order to understand the influences of modifications of the reactor configuration and material on the microdischarges.[3] Until recently, only a few researchers focused on numerical studies dealing with DBD. Eliasson and Kogelschatz[6] showed information on a single microdischarge combined with reaction chemistry in a single barrier reactor. Another study, by Kang et al.,[7] presented a numerical study for understanding the influences of barrier arrangements on the evolution and characteristics of discharges in a DBD. The motions of electrons, positive ions, and negative ions in DBD were described by a set of continuity equations. The model includes the direct interactions of electrons and photons with neutral gas particles, such as electron impact ionization, electron attachment, and photon impact ionization. However, it is rare to find comprehensive plasma modeling in a DBD reactor in relation to optimization of process parameters, which is vital in industrial applications. Comprehensive plasma reactor modeling should take into account various points of view, such as chemistry, chemical reaction and kinetics, catalysis, and physics. Accordingly, the plasma model becomes very complex.

Artificial neural networks (ANNs) have been widely used in chemical engineering applications for complex process modeling, process control, and fault detection and diagnosis.[8−11] Meanwhile, the combination of ANN and genetic algorithm (GA) has been used for integrated process modeling and optimization.[12−14] The hybrid ANN−GA technique is a powerful method for process modeling and optimization that is better than other techniques such as response surface methodology, particularly for complex process models. The phenomenologically comprehensive plasma reactor model needs a robust numerical solver and is time-consuming to solve, which is not suitable for rapid prediction in optimization and process control. Artificial neural network (ANN) modeling is chosen to model the complex behavior between input and output in the DBD plasma process, either without or with a catalyst. Therefore, the development of a robust hybrid ANN−GA algorithm is necessary to simulate the plasma reactor.

The present contribution is intended to develop an integrated algorithm of artificial neural network−genetic algorithm (ANN−GA) to facilitate modeling and optimization of a DBD plasma reactor. The integrated approach is intended to simplify the complex process model particularly in the DBD plasma reactor. Multiobjectives optimization is implemented to obtain optimal operating parameters and maximum reactor performances.

2. Experimental and Numerical Methods

2.1. Apparatus of DBD Plasma Reactor. The experimental apparatus of a DBD plasma reactor is schematically depicted in Figure 1, while the configuration or design of the DBD plasma reactor is displayed in Figure 2. A high-voltage ac generator supplying a voltage from 0 to 17.5 kV with a pulsed waveform at a frequency of up to 10 kHz was used. The voltage measurement was conducted using an oscilloscope (ISO-TECH ISR 622) equipped with a high-voltage probe (manufactured by Atama Tech Sdn. Bhd.). Atama's high-voltage probe was calibrated using a Tektronix P6015 high-voltage probe. The circuit for a high-voltage pulse ac generator as depicted in Figure 3 can be divided into two main sections: the oscillator and the power drive. The oscillator was built around a CMOS 4093 (4-nand gates) and was configured as a pulse generator (duty

* To whom correspondence should be addressed. Tel.: +62-24-7460058. Fax. +62-24-7460058. E-mail: istadi@tekim.ft.undip.ac.id.
† Diponegoro University.
‡ Universiti Teknologi Malaysia.

10.1021/ie060562c CCC: $33.50
Published on Web 09/02/2006