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# Optimization Control of Coal Methanol Chemical Process Based on Neural Network Algorithm

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Nowadays, the world has become a unified factory. However, with the adoption of coal resources gradually increased, the waste of coal resources and environmental pollution has increased. Under such occasion, methanol as an alternative energy source plays a more prominent role in the economy. But, the process and equipment of coal-to-methanol are far from perfect, which directly leads to the result that the adoption of coalto-methanol technology is disadvantageous and lacks of development. Therefore, the production process of coal to methanol requires the following economical design. First, the coal should be saved through the intelligent improvement and the optimization of process, so as to continuously improve the efficiency of the process. Secondly, in the process of coal to methanol, electric energy should be saved. Through the renewal of equipment, the energy consumption can be continuously saved. The real-time optimization control method can solve the problem of optimization and control the complex process industry, so as to make the process run as economically optimized as possible. Besides, the on-line learning ability of neural network makes it a unique advantage in on-line controller, and hence, it is an important tool for real-time optimization control. This paper makes full use of the advantages of neural network algorithm to optimize the process production of coal-to-methanol. First of all, the process of coal to methanol is mainly focused on, and the key links of the production process are introduced. Secondly, the neural network algorithm is studied. Then, a control method based on neural network algorithm is proposed for real-time optimization control of coal-to-methanol production. Finally, in the simulation experiment, the proposed method is verified and analyzed. Experimental results show that the control method of neural network algorithm can make sure the smooth operation of coalto-methanol production process, and realize a high control precision. When the efficient production conditions can be guaranteed, the energy consumption of the system can also be effectively reduced. Similarly, the energy saving effect is guite remarkable.

# 1. Introduction

In the past ten years, with ethylene serving as its representative, the modern oil industry is developing rapidly. However, as there is a shortage of oil resources soon, the dependence of oil on other material continues to increase. With the development of economy and the lack of energy in the world, all the countries in the world are looking for new alternative energy. As a new energy, methanol can not only improve the deterioration of the world environment, but also bring a glimmer of hope for the world energy crisis. At present, 80% of the world's methanol production raw materials are from natural gas line. Nevertheless, from the perspective of the long term development, coal is the largest reserves of fossil energy resources in the world, which is far more than the storage amount of oil and gas. As the technology of gasification and purification develops rapidly, methanol is applied as a clean alternative energy, which makes the methanol that is produce by coal as the main raw material gas for methanol synthesis route.

Shell coal gasification technology is a pulverized coal gasification process with pressurized gas flow bed, which is developed by Holland International Petroleum Corporation. The gasification agent is oxygen, and the slag is discharged from the hearth in liquid form. Since 1954, the world's first set of low temperature methanol washing devices is built in the South Africa Company's fuel plant. Now the Low temperature Rectisol Process

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has a development history of 60 years. Chen (2005) has developed the RPS software which is specially used for the simulation of low temperature methanol washing system and suitable for Windows operation platform. It makes the operation interface friendlier, and also makes it easier to understand and more professional. Zhang J. T. (2010) proposes a five-tower methanol distillation process, adding a medium pressure column between the four tower process of the traditional pressure and atmospheric tower. This method realizes a multi-effect distillation, and reduces the energy consumption to 33.6%. Wu (2005) puts forward a new three-tower rectification process. On the basis of the traditional three tower process, the material was collected from the feed line above the pressure tower, which is made as the feed of the atmospheric tower. Douglas, A., P. (2006) and other people have compared the energy consumption and economic benefits of the Twin Towers, the three towers and the thermally coupled three tower distillation process by analyzing the total combined curve of the tower (CGCC) and the system total combined curve (GCC).

As a natural computing technology, artificial neural networks have been widely used in many fields, such as control, prediction, optimization, system identification, signal processing and pattern recognition, and so on. (Zhao et al., 2011)). Cellular Neural Networks (CNNs), which is proposed by Chua and Ling in 1988, is a representative of the Hopfield model (Chua et al., 1988)). Abbass (2002) uses weight training algorithm, which is based on BP algorithm and differential evolution algorithm, to improve neural networks and predict breast cancer. Lionen (2003) uses differential evolution algorithm to train the weights of feed-forward neural network, and compares it with the gradient descent neural network training method. The results show the effectiveness of DE algorithm.

This paper makes full use of the neural network algorithm to optimize the process of producing coal methanol. First of all, in this paper it focuses on the process of transferring coal to methanol, and introduces the key parts of production process. Secondly, the neural network algorithm is studied. Then, a control method based on neural network algorithm is proposed for real-time optimization control of transferring coal to methanol. Finally, in the simulation experiment, the proposed method is verified and analyzed. In the Experiments, it is show that the control method based on neural network algorithm can ensure the smooth operation of transferring coal to methanol, and achieve high control precision. While ensuring efficient production conditions, it can effectively reduce the energy consumption of the system, and the energy saving effect is remarkable.

# 2. Study on coal-to-methanol process

Methanol is an important clean liquid fuel and organic chemical raw material. It is widely used in fuel, organic synthesis, medicine, pesticide, coating and national defence industry. Solid raw material, coal, liquid raw material, naphtha, gas raw material, natural gas, coal bed gas, and oil field gas can be transformed to the syngas by means of steam reforming K or partial oxidation. The main components of syngas are H2 and CO, which can be produced by W under the action of catalyst. Since the p methanol and its derivatives are widely used all over the world, methanol has been regarded as an important research area of carbon chemical industry. At present, methanol has become an important starting material for the new generation of energy, which can produce a series of deep processing products, and become a breakthrough in carbon chemical industry. On the occasion of lacking oil resources and requiring environmental protection, methanol is made with W coal as the raw materials, which is expected to become the implementation of the clean use of coal, and make up for the oil energy shortage. So the methanol chemical industry has become one of the main fields of chemical industry and energy industry. Figure 1 is the flow chart of coal methanol plant.



Figure 1: The flow chart of coal methanol plant

## 2.1 Basic properties of methanol

Methanol is the simplest molecular structure of aliphatic alcohols. It can be miscible with water, ethanol, ether and many other organic compounds, but its solubility in aliphatic hydrocarbons is very low. Methanol is easy to absorb water vapour, CO<sup>2</sup>, SO<sup>2</sup>, H<sup>2</sup>S and other substances, so it is difficult to obtain completely anhydrous methanol. It is composed of methyl and hydroxyl with a simple and polar structure, which makes its chemical properties very lively. Many important chemical products can be synthesized through the oxidation and

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substitution of hydroxyl groups, such as formaldehyde, formic acid and dimethyl ether. In addition, methanol itself can be used as fuel and it is widely used in many fields.

(1) Methanol as fuel (Li et al., 2008; Wu et al., 2007; Li, 2003)

Methanol fuel has three main applications. First, it is used as the fuel for motor vehicles. Second, it is used as fuel cells. Third, it is used as domestic fuel.

(2) Methanol- to-formaldehyde and paraformaldehyde

Formaldehyde is one of the most important derivatives of methanol. Poly-formaldehyde is the further extending production of industrial chain products after methanol is transformed to formaldehyde, which is one of the three largest general thermoplastic engineering plastics in the world. It is widely used in automobile making, electronics, electrical machinery manufacturing, building materials and other fields. Figure 2 is a process for transferring methanol to paraformaldehyde.



Figure 2: The process flow sheet of methanol to polyformaldehyde

## (3) Methanol ester derivatives

The esterification of methanol with organic acids (such as formic acid, acetic acid, etc.) or inorganic acids (such as sulphuric acid, phosphoric acid, etc.) can produce ester derivatives. These ester derivatives mainly include methyl format, dimethyl sulphate, methyl-carbonate, phosphoric acid trim-ethyl ester and phosphate ester and so on.

(4) Methanol production of amines and other derivatives

The amine derivatives of methanol are mainly produced by substitution and acylation. They are widely used in perfumes, dyes, pharmaceuticals, pesticides, national defence, chemical and other fields. Using the vapour ammonification method of producing methylamine by methanol as an example, in the situation of  $420^{\circ}$ C and 4.9MPa,the substitution of methanol with ammonia happens under the action of catalyst. Then the mixture will be replaced, and the mixture goes into the subsequent separation process so as to get the qualified methylamine products. The reaction equation is as follows.

$$CH_3OH + NH_3 \rightarrow CH_3NH_2 + H_2O \tag{1}$$

$$2CH_3OH + NH_3 \rightarrow (CH_3)_2NH_2 + 2H_2O \tag{2}$$

$$3CH_3OH + NH_3 \rightarrow (CH_3)_3NH_2 + 3H_2O \tag{3}$$

## (5) Methanol derivatives of acids

Acetic acid is commonly known as acetic acid. It is an important basic chemical raw material, which can be used in chemical industry, light industry, metal processing, medicine, pesticides, and explosives and so on. (6) Hydrocarbon derivatives from methanol

The alcohol based hydrocarbon derivatives mainly consist of two major directions. They are methanol to gasoline (MTG) and methanol to olefins.

#### 2.2 Preparation process of coal-to-methanol

The production of coal methanol process includes four main processes, which are gas, purification, synthesis and purification. The ratio of oxygen to carbon and water gas ratio of crude syngas produced by different coal gasification technologies are not the same. The gasification technology determines the technical route of the transformation unit, the whole plant steam balance and the waste heat utilization plan of the process. Therefore, the determination of the technical scheme of the coal to methanol system mainly depends on the selection of the technical scheme of coal gasification. Gasification technology is the basic technology of coal chemical industry. As the leading technology unit of coal methanol device, it has the characteristics of high input, and high reliability. According to the different contact ways between coal and gas agent in furnace, the coal gasification methods can be divided into three types, which are fixed bed, fluidized bed and gas flow bed.

The methanol synthesis process is the core unit of the methanol synthesis process, and the key parts are the methanol synthesis catalyst and reactor. The catalysts for methanol synthesis mainly include five kinds of catalysts: zinc chromium, copper base and palladium series, molybdenum series and low temperature liquid phase. Methanol synthesis gas has a hydrogen/carbon ratio of about 2 after coal gasification, conversion, and purification. It firstly goes through the combined compressor to increase the pressure to 5.78 MPa, and preheats it to 225. Then it enters the top of methanol synthesis tower, which is divided into two parts, the upper and lower parts. The upper and lower helical tubes are filled with methanol synthesis catalysts. Under its catalysis, the active component in the synthesis gas reacts with methanol to produce methanol and emits a large amount of reaction heat. Methanol synthesis process mainly has three kinds, which are low pressure method, medium voltage method and high pressure method. Low pressure method and medium pressure method are mainly used in industrial production, while high pressure method is gradually phased out due to its harsh operating conditions, investment and production cost. More than 80% of the total amount of methanol in the world is produced by low pressure method and medium pressure method.

Production of methanol synthesis is the original methanol which contains light components like two dimethyl ether, alkanes, carbonyl compounds, and heavy constituents like water, ethanol and other advanced alcohols. In order to produce standard fine methanol, the original methanol will be purified by distillation. The common methanol rectification processes are single column distillation, Twin towers rectification, triple column rectification and four column distillation.

## 3. Neural network research

An artificial neural network is a self-organizing, nonlinear, and adaptive system which is made up of some simple neural processing units. It is a structure similar to the synaptic connections of the brain. And it simulates the human nervous system to make a mathematical model for processing, memorizing, and processing information.

## 3.1 Neural network classification

Neural networks are networks that are interconnected by a large number of neurons. According to the different connection modes, neural networks can be divided into two major categories, which are forward feed networks without feedback and feedback networks. The correspondence between the neuron output Y and the input X can be expressed as follows.

$$Y = f(\sum_{j=1}^{r} w_j x_j + a) = f(W * X + a)$$
(4)

At present, there are many different models of neural networks. Forward networks include perceptron, BP networks, GMDH networks, and RBF networks. The feedback network includes network CG model, box midbrain (BSB) model, Hopfield network model, bidirectional associative memory, regression BP network and Boltzmann network.

#### 3.2 Basic structure of neural network

Artificial neuron model is the simulation and abstraction of biological neuron. The abstraction here is talked from the mathematical point of view. The so-called simulation is based on the structure and function of neurons.

By repeatedly running between multilayer structures of the neural network, the correct rate of input mode continues to improve. When it reaches the range of permissible error or the training number reaches the predesigned number, the training process will come to an end.

### 4. Optimal control study on coal methanol process based on neural network algorithm

The conversion reaction of carbon monoxide and water vapor is an essential process for the synthesis of ammonia, methanol and hydrogen by the synthesis of coal and gas by using coal as the raw material. The main purpose of the transformation process is to transfer CO to  $H_2$ . However, the total change is influenced by the factors such as process setting, process parameters, catalyst loading, total conversion gas, reaction temperature and other process factors. The bottom evaluation index of the real-time optimization control of the transformation process is mainly to evaluate the tracking performance of the loop level controller (such as the control accuracy, and the control fluctuation, etc.). The CO potency in the converting reactor outlet of the transformation process is a very important control variable. According to the design method of the traditional neural network controller, a neural network controller is set up as for the concentration control.

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The functional relationship is established, which is between the transformation input model X and the output model Y. As for a neural network with HLN (Hidden Layer Neurons), as long as its function has a limit at one of its infinity, it can approach any sample of any N dimension with zero error. Moreover, the forward feed neural network trained by BP algorithm is also proved to have a strong convergence. Therefore, by using the approximation characteristics of neural networks, a modelling neural network can be designed to model the CO transformation system. According to the modelling neural network, the structure and characteristics of the neural network can be adopted to determine the functional relationship between X and Y. At the same time, we design a neural network controller to control the exit concentration using the on-line learning ability of neural networks. The hidden layer transfer function adopts Sigmoid function, which satisfies the requirement of activation function of neural network in theorem. Fig.3 shows the thought of the designed neural network modelling and control.



Figure 3: The structure of the designed neural network modelling and control

The neural network controller is designed for the nonlinear characteristics of the CO concentration at the converter outlet, which aims to achieve the high precision control of the concentration. The method is to set the error E(k) = r-y(k), which is the error between the system actual output and the CO setting concentration, as the input of the neural network controller. At the same time, the output of the neural network controller isset as the variation of CO concentration control K, so as to control the CO concentration. The output of the neural network controller is as follows.

$$u(k) = J_2^c(k) f(J_1^c(k)e(k))$$

(5)

In this formula,  $J_1^c(k)$  is the connection weight matrix, which lies between the input layer of the neural network controller and the hidden layer. Besides,  $J_2^c(k)$  represents the connection weight matrix between the hidden layer of the neural network controller and the output layer.

Using the characteristics of neural networks such as self-optimization and constraint convergence, this paper accurately controls the export of CO, and provides a new method for improving methanol production and energy consumption control.

# 5. Experiment and Analysis

## 5.1 Experiment design

Most of the coatings quickly absorb water when they are exposed to wet conditions or soaked in water. When water enters the coatings and reaches the metal matrix, electrolyte solution will be formed and cover the surface of the metal, which leads to corrosion reaction of the metal matrix. Therefore, it is an important index to evaluate the corrosion resistance of the coatings by studying their electrochemical corrosion of the medium to the base metal. In this paper, we have designed a test compared with the common anticorrosive paint sold on the market. The corrosion mediums are 3.5%NaCl, 10%NaOH and 10%H2SO4 respectively.

## 5.2 Experiment Results and Analysis

Based on the production data of a factory under different temperature and flow rate, catalyst volume and other conditions, the simulation experiments are made. The simulation software is the MATLAB. R2010b platform, with the Intel quad core CPU as the experimental operation computer, and 3.4GHas the dominant frequency.

As can be seen in Table 1, the improved method can greatly enlarge the production of methanol, and the corresponding energy consumption is also effectively reduced.

Projects	Traditional process	Improved process
Compressor power consumption(kW)	530	473
CO <sub>2</sub> concentration (%)	97.321	98.899
Recovery of CO <sub>2</sub> (%)	19.36	48.71

	Table 1:	The	results	of	anti-chemical	corrosion	text
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# 6. Conclusion

The new method makes full use of the advantages of neural network algorithm and optimizes the production process of coal methanol. First of all, it focuses on the process of coal-to-methanol, and then introduces the key parts of production process. Secondly, the neural network algorithm is studied. Then, we propose a real-time optimization control method for coal and methanol production based on neural network algorithm. Finally, we carry out the experiment. Through experiments, it is proves that the control method of neural network algorithm can guarantee the smooth operation of coal-to-methanol production process, and also achieve a high control precision. At the same time, while ensuring high production efficiency, it can also effectively reduce the energy consumption of the system, and simultaneously have a remarkable energy saving effect.

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