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A Knowledge Base System for Operation Optimization: Design and Implementation Practice for the Polyethylene Process

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ABSTRACT

Setting up a knowledge base is a helpful way to optimize the operation of the polyethylene process by improving the performance and the efficiency of reuse of information and knowledge—two critical elements in polyethylene smart manufacturing. In this paper, we propose an overall structure for a knowledge base based on practical customer demand and the mechanism of the polyethylene process. First, an ontology of the polyethylene process constructed using the seven-step method is introduced as a carrier for knowledge representation and sharing. Next, a prediction method is presented for the molecular weight distribution (MWD) based on a back propagation (BP) neural network model, by analyzing the relationships between the operating conditions and the parameters of the MWD. Based on this network, a differential evolution algorithm is introduced to optimize the operating conditions by tuning the MWD. Finally, utilizing a MySQL database and the Java programming language, a knowledge base system for the operation optimization of the polyethylene process based on a browser/server framework is realized.

1. Introduction

Due to significant development in the field of modern information technology, the traditional manufacturing industry is facing severe challenges, and urgently requires upgrading and transformation through advanced information technology. Accordingly, industrialized countries have proposed policies such as the corresponding initiative in China and Industry 4.0 [1]. Naturally, as a typical traditional industry, the petrochemical industry will benefit from these initiatives, which will generate new demands and opportunities [2].

The corresponding initiative in China strongly focuses on smart manufacturing, which involves the application of artificial intelligence and network technology—such as advanced process control and real-time optimization—to traditional manufacturing information systems [3]. Zhuang et al. [4] previously proposed conflict prediction based on fuzzy temporal knowledge reasoning, which can provide helpful information for use in train operation adjustment and train timetable improvement. Regarding semantic representation of equipment, Yu et al. [5] proposed a method to display and analyze equipment knowledge. Due to the increasing number of reusable solutions on the electronics market, Subbotin et al. [6] designed a knowledge base recommendation system to help developers select a hardware–software platform for embedded systems automated design. Although knowledge representation and reasoning are applied in many research fields, their use is less common in industrial plants. Compared with conventional manufacturing, smart manufacturing provides the opportunity to analyze the various influencing factors of an operation by combining intelligent technologies in depth, such as big data processing and neural network-based modeling. Smart manufacturing can also adjust the operating conditions and production plan to realize flexible and efficient production. Thus, it enables industrial plants, especially in the petrochemical industry, to make timely adjustments according to market demand and process status, thereby improving their market competitiveness. In order to enhance the reuse of manufacturing knowledge, the knowledge base system has been introduced into the field of industrial manufacturing and applied in some simple, discrete manufacturing fields [7,8].

However, there is no universal framework for domain knowledge for the polyethylene process at present, either in the literature or on the market, due to its complex reaction mechanisms, various types of polyethylene products, and flexible production process. The selection of different equipment and production designs for the polyethylene production process results in different

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choices for the parameters of the molecular weight distribution (MWD) calculation, which require many rules known only to experts. Particularly for the optimized operation of the production process, it is necessary to recalculate the optimized operating parameters for each optimization calculation. In this calculation process, experiences accumulated by experts cannot be effectively utilized. Solving the problem of expert experience knowledge reuse is key in improving production intelligence. Consequently, this absence restricts not only the sharing of polyethylene operation knowledge, but also the development of smart manufacturing in the polyethylene industry.

The knowledge base system has been applied effectively to equipment selection for the styrene process [9], which indicates a promising possibility of application to the polyethylene process as well. Hence, in this paper, we introduce the techniques of the domain knowledge base to the polyethylene industry and propose a framework of a domain knowledge base for the polyethylene process. Using this framework as a basis to integrate the knowledge of the polyethylene process, equipment operation, and operation optimization, we propose an operation optimization knowledge base system (OOKBS) for a practical polyethylene process.

2. System architecture of the OOKBS

The structure of the OOKBS for the polyethylene process contains three layers, where each layer is designed to focus on specific tasks to facilitate the operation of higher layers. Fig. 1 provides a diagram of the structure of the OOKBS.

The bottom layer is the ontology layer, which consists of the polyethylene ontology, expert rules for the polyethylene process, and ontology reasoning and analysis. The polyethylene ontology describes polyethylene process-related knowledge, such as chemical equipment, optimal operation conditions, and operation variables. The expert rules preserve past experience related to parameter selection for optimization calculations of molecular weight under various process conditions. The ontology reasoning and analysis provide the recommendation capability to select suitable operation parameters for the optimized MWD based on the real-time production status.

The middle layer is the model layer, which comprises the polyethylene process model, along with the prediction and optimization algorithms for the MWD of the polyethylene process.

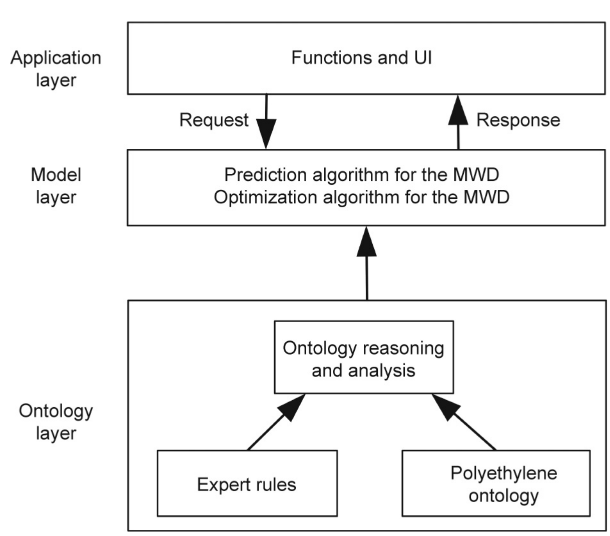

Fig. 1. Architecture of the operation optimization knowledge base system (OOKBS). UI: user interface.

The top layer is the application layer, which provides knowledge application services to users, including an information overview service, an operation optimization service, and a user management service.

3. Construction of the ontology of the polyethylene process

In this section, the definition and attributes of the ontology of the polyethylene process are given, and a construction method is introduced based on the characteristics of the polyethylene production domain knowledge.

3.1. Description of ontology

Ontology is an important tool representing knowledge and concepts; it can describe domain objects and corresponding interrelationships and rules [10]. With the development of information technology, the idea of ontology was introduced into the field of informatics, and researchers have given new meanings to ontology.

Since an ontology is simply a description of a specific domain, there is no universal method for ontology construction. Therefore, a common method is to manually construct it according to the specific demands of the corresponding application.

Examples of commonly applied manual construction methods include the seven-step [11], Enterprise Ontology [12], Toronto Virtual Enterprise (TOVE) [13], METHONTOLOGY [14], and KACTUS [15] methods. The Enterprise Ontology and TOVE methods focus on enterprise and commercial activities. Implementation of the METHONTOLOGY and KACTUS methods is complex, and lacks effective tool support. In most cases, the seven-step method is simpler and more effective than other ontology modeling methods, and is more suitable for building a domain ontology with a Jena application programming interface (API) [16]. The seven-step method was originally proposed by Natalya F. Noy and Deborah L. McGuinness to solve ontological construction problems, and has been applied to chemical equipment-related description and reasoning [11,17]. Hence, the seven-step method is used for ontology modeling in this work.

3.2. Construction of the ontology of the polyethylene process

Considering the aforementioned characteristics of the polyethylene process domain knowledge, the seven-step method was adopted to construct an ontology of the domain knowledge.

As the ontology library must cover polyethylene process-related knowledge, the ontology of the polyethylene process is divided into five subclasses: chemical equipment, product craft, polyethylene types, variables, and optimal conditions.

(1) Chemical equipment. This class defines the equipment involved in the ethylene polymerization reaction, such as the reactor and transmission equipment, as listed in Table 1.

(2) Product craft. This class describes the polyethylene process, which can be divided into four types of process. Each process method consists of many cell process methods. Table 2 presents the class hierarchy of the polyethylene process.

Table 1
Chemical equipment class.

Parent class	Child class
Chemical equipment	Reactor Transmission equipment Heat-exchange equipment Recycling equipment Product tank Mass transfer

Table 2
Product craft class.

Parent class	Child class
Product craft	Vapor process Slurry process Solution process High-pressure process

(3) Polyethylene types. This class describes the type of polyethylene product. Different polymerization schemes produce various types of polyethylene products. Based on the density distribution range, polyethylene products can be divided into high-density polyethylene (HDPE), medium-density polyethylene (MDPE), low-density polyethylene (LDPE), and linear low-density polyethylene (LLDPE), as listed in Table 3.

(4) Variables. This class describes the control variables and product quality indexes used in the polyethylene process. It contains the hydrogen feed quantity (f_{H_2}), ethylene feed quantity ($f_{C_2H_4}$), butene feed quantity ($f_{C_4H_8}$), temperature, pressure, mole ratio of hydrogen to ethylene (m_{H_2}/m_{C_2}), and mole ratio of butene to ethylene (m_{C_4}/m_{C_2}). The quality indexes of the products include the melt index, density, and MWD. Table 4 shows the structure of the variable class.

(5) Optimal conditions. This class defines the optimal operating conditions of the operation optimization class. The structure of this class is provided in Table 5.

Table 3
Polyethylene type class.

Parent class	Child class
Polyethylene type	HDPE MDPE LDPE LLDPE

Table 4
Variable class.

Parent class	Child class
Control variable	Reactor temperature Reactor pressure f_{H_2} $f_{C_2H_4}$ $f_{C_4H_8}$ m_{H_2}/m_{C_2} m_{C_4}/m_{C_2}
Quality index	Melt index Density MWD

Table 5
Optimal conditions class.

Parent class	Child class
Optimal condition	OP of reactor temperature OP of reactor pressure OP of f_{H_2} OP of $f_{C_2H_4}$ OP of $f_{C_4H_8}$ OP of m_{H_2}/m_{C_2} OP of m_{C_4}/m_{C_2}

OP: operating point.

3.3. Construction of ontology attributes

The Web Ontology Language (OWL), which is an ontology description language standard, has two main property types: data property and object property. Object property is usually used to represent the relationship between instances, whereas data property is usually utilized to represent the data properties that an object possesses. Based on the core concept glossary for chemical field equipment, Table 6 presents the data properties and Table 7 lists the object properties.

3.4. Ontology storage

After the reasoning and analysis of the ontology of the polyethylene process is complete, the information obtained from the analytical results must be stored. The OWL can be stored using three methods: professional management tools, plain text, and a database system. To facilitate the integration of the system, a MySQL database was utilized to store the ontology information, while a Jena API was used to provide a rationale and analyze the ontology.

4. Prediction and optimization of polyethylene MWD

In this section, the polyethylene MWD is defined based on the relative quantity of different molecular weight polymers. Prediction and optimization of the polyethylene MWD is illustrated [18,19].

4.1. Description of polyethylene MWD

The MWD is the relative quantity distribution of each different molecular structure in the polymer. The relative quantity is based on a probability function, which can usually be fitted by the distribution function. As the Schulz–Flory distribution is applicable to describe the MWD of a linear poly-condensation [20], it is often used to calculate the chain length distribution generated at a certain active site. The Schulz–Flory distribution can be modeled as follows:

$$w_r(j) = r\tau(j)^2\exp(-r\tau(j)) \quad j = 1, 2, \ldots, N \tag{1}$$

where N is the number of active sites of the catalyst; $w_r(j)$ is the molecular chain length distribution of polyethylene; r is the molecular chain length of polyethylene; and $\tau(j)$ is the ratio of the chain transfer rate to the chain growth rate, also known as the distribution

Table 6
Data property

Domain	Data property	Range
Chemical equipment	Has pressure	Float
Chemical equipment	Has temperature	Float
Variable	Has flow	Float
...	...	...
Optimal condition	Has value	Float
Variable	Increase value	Float
Variable	Decrease value	Float

Table 7
Object property

Domain	Object property	Range
Control variable	Affect	Product craft
Product craft	Produce	Polyethylene type
Polyethylene type	Apply process	Product craft
Variable	Happen in	Chemical equipment

function parameter. By mathematical transformation, the above formula can be written in the following logarithmic form:

$$w_{\log \mathrm{MW}}(j) = 2.3026\left(\frac{\mathrm{MW}}{\overline{\mathrm{M}}_n(j)}\right)^2 \exp\left(-\frac{\mathrm{MW}}{\overline{\mathrm{M}}_n(j)}\right) \tag{2}$$

where $w_{\log\mathrm{MW}}(j)$ is the logarithmic expression of $w_r(j)$, $\overline{M}_n(j)$ is the average molecular weight, and MW is the molecular weight of polyethylene.

We take the Ziegler–Natta catalyst as the polymerization catalyst. It has multiple active sites, and the MWD of each active site is subject to the Schulz–Flory distribution. The logarithmic MWD formula of polyethylene is obtained by superimposing the MWD of each active site as follows:

$$w_{\log\mathrm{MW}} = \sum_{j}^{N} m(j) w_{\log\mathrm{MW}}(j) \quad j = 1, 2, \ldots, N \tag{3}$$

where $m(j)$ is the weight of the jth active site in the distribution function.

4.2. Prediction of polyethylene MWD

Considering the complex structure of polyethylene products, state-of-art modeling and detection methods for MWD are not effective enough. Among these is gel permeation chromatography; however, although this method can be used to detect polyethylene products offline, it cannot reflect product performance in real time and is not conducive to the online optimization control of product quality. A model based on the MWD mechanism will be more accurate and will solve the problem of MWD online prediction.

The influencing factors are analyzed based on the cumulative distribution function (CDF) of the polymer. A model is then established based on the relationship among the operating conditions, the parameters, and the weights of the distribution function. Fig. 2 depicts a diagram of the modeling process. In the upper part, a back propagation (BP) neural network model is used to train the data under the reactor operating conditions in order to obtain the model. In the lower half of the diagram, based on the model generated in the upper part, the MWD is calculated based on the actual operating conditions.

A neural network model of the polyethylene MWD is established to obtain the relationship between the operating conditions and the parameters of the MWD. This relationship can be obtained by combining the distribution function parameters obtained from the model with the MWD function.

Because a cross analysis between the analysis model data and industrial data can improve the MWD prediction, datasets of these variables for ethylene polymerization using the Aspen model and a historical production database were collected, and 500 datasets were selected. Table 8 lists the input variables for the model.

Four active sites of the catalyst in this polymerization system are selected as the input variables, and the distribution of molecular weight of the Aspen model and sample is analyzed to obtain the distribution function parameters, which are used as the output of the neural network. Therefore, the output variable Y of the model is defined as $Y = [p^1, p^2, p^3, p^4]$ (p: parameter).

We select 85% of the data from the 500 datasets in the sample set as the training sample. The remaining 15% of the sample data (75 datasets) is used as test samples to verify the model. A BP model is used to establish the model between the operating conditions and the parameters of the MWD, in order to obtain the relationship between the operating conditions and the parameters. The MWD can be predicted by combining the distribution function with the above results.

Fig. 3 shows a comparison between the test values analyzed from the sample and the predicted values from the four distribution function of the model parameters. In the polyethylene production process, the MWD is only related to the distribution function parameters. The parameters of the four subfigures in Fig. 3 correspond to p^1, p^2, p^3, and p^4 of the output variable Y of the model, as defined above. It can be seen that the predicted value curve calculated by the model fits well with the value curve analyzed from the sample. Therefore, by establishing a model between the production variables and the distribution function parameters, the MWD can be predicted.

4.3. Optimization of polyethylene MWD

The optimization problem of the MWD is described as follows: based on a given expected MWD, suitable production conditions of polyethylene is found such that the MWD of the polyethylene products produced under these conditions is the closest to the expected distribution (expressed as $\overline{\mathrm{MWD}}$ in Eq. (4)).

The MWD of polyethylene is a curve, which is divided into 100 sample points. The objective function for the optimization problem of MWD is

$$\min \sum_{i=1}^{100} \left(\mathrm{MWD}_i - \overline{\mathrm{MWD}}_i\right)^2 \tag{4}$$

Table 8
Input variables for the model.

Variable	Description	Unit
$f_{C_2H_4}$	Ethylene feed	$kg \cdot h^{-1}$
$f_{C_4H_8}$	Butene feed	$kg \cdot h^{-1}$
f_{H_2}	Hydrogen feed	$kg \cdot h^{-1}$
m_{H_2}/m_{C_2}	Mole ratio of hydrogen to ethylene	$mol \cdot mol^{-1}$
m_{C_4}/m_{C_2}	Mole ratio of butene to ethylene	$mol \cdot mol^{-1}$
T	Reaction temperature	°C
P	Reaction pressure	MPa

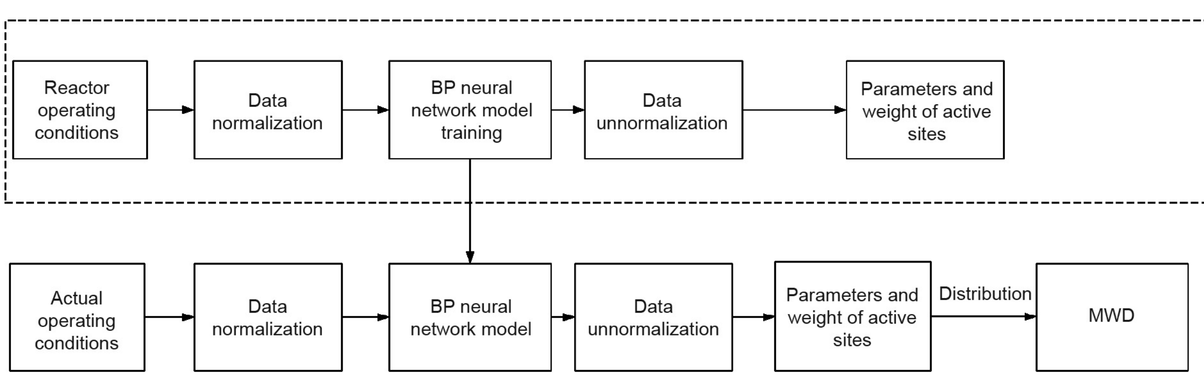

Fig. 2. Diagram of the MWD modeling process. BP: back propagation.

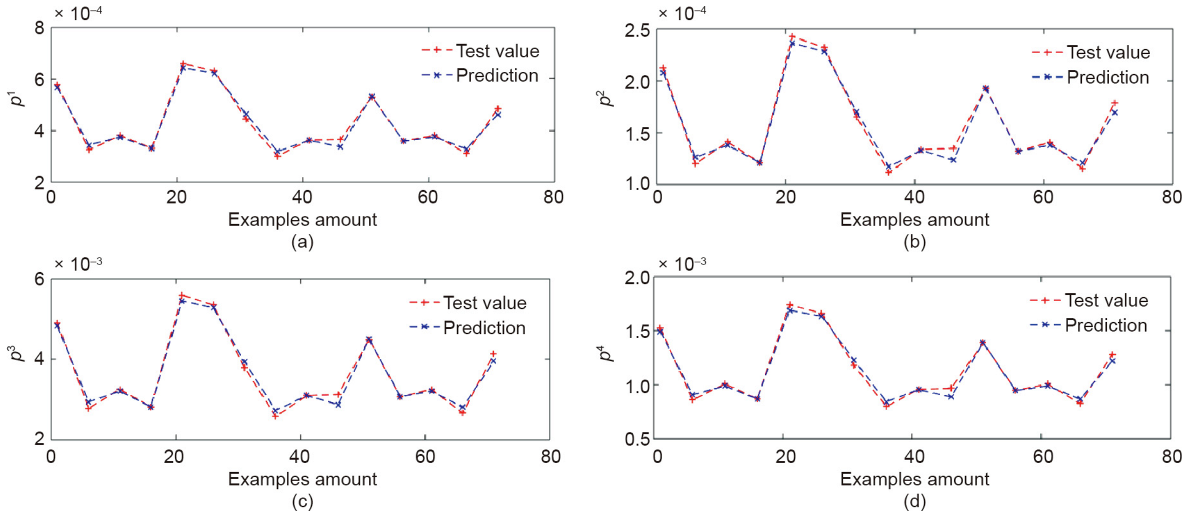

Fig. 3. Comparison between the test values and the model's predicted values of the parameters. (a) Curve for p^1; (b) curve for p^2; (c) curve for p^3; (d) curve for p^4.

where MWD_i is the value of the optimized polyethylene MWD curve at sample point *i*, and $\overline{MWD}_i$ is the value of the expected polyethylene MWD curve at sample point *i*.

Differential evolution algorithms can be applied to this MWD optimization problem. Table 4 lists the decision variables of the optimization problem. In order to achieve better results, based on the expert rules of the ontology layer, the main parameters of the differential evolution algorithm are set as follows: population size *NP* is set to 50, mutation operator *F* is set to 0.5, and crossover probability *CR* is set to 0.8.

Based on the prediction model of the polyethylene MWD, the difference between the expected MWD and the optimal MWD is minimized using the differential evolution algorithm. Fig. 4 shows a comparison between the optimized polyethylene MWD curve and the expected polyethylene MWD curve when the optimization operation is completed, where d*W*/dlgMWD is the probability density distribution function of molecular weight. The expected polyethylene MWD curve is basically consistent with the optimized polyethylene MWD curve. Thus, the optimization of the differential evolution algorithm on MWD is satisfactory.

5. Implementation of the OOKBS

The construction, reasoning, and analysis of the ontology library of the knowledge base system, in addition to the prediction and optimization of the polyethylene MWD, provide support for the application of the OOKBS for the polyethylene process. Based on

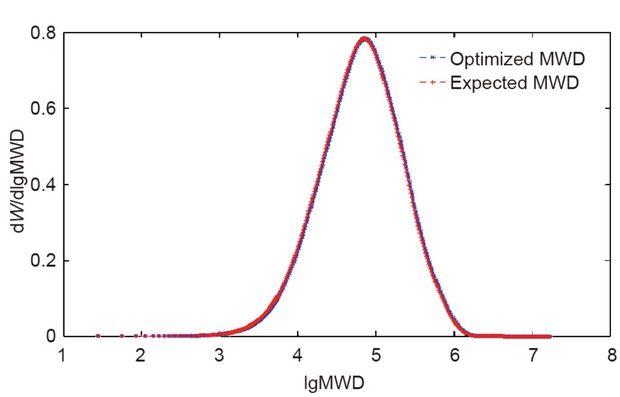

Fig. 4. Comparison between the optimized polyethylene MWD curve and the expected polyethylene MWD curve.

the requirements obtained from optimizing the polyethylene process, the system performs the following functions:

(1) The OOKBS provides knowledge management of the polyethylene process, including information on equipment, raw material, and the process.

(2) The OOKBS autonomously extracts the rules from experiences accumulated by experts, production manual, technical specification, and relevant technical literature in the field of the polyethylene process. It also provides logical reasoning-based rules.

(3) According to the operating condition data inputted by a user, the OOKBS can predict the MWD of the product corresponding to the operating conditions. Based on the expected MWD data uploaded by the user, the system can provide optimized working conditions using the optimization algorithm.

(4) The OOKBS provides system maintenance, database management, and user management, in addition to a user behavior record to ensure system security.

5.1. Functions of the OOKBS

The application layer of a knowledge base system is the human–computer interface of the system. To improve the system accessibility and scalability, this layer is developed using browser/service architecture.

There are three main functions of the system: information overview, operation optimization, and user information. Information overview mainly evaluates information on the equipment, raw materials, and production process. Operation optimization consists of the process flow, model information, expert information management, exception information, and MWD optimization. User information primarily provides user management and an operation log view. Fig. 5 depicts the structure of the application layer.

5.2. Structure of the OOKBS database

To improve system availability, the application database is designed to store product information, rules, MWD data from experts, and other information.

(1) Product information. To address the issues related to integrating the data analysis with the association analysis of the equipment and the historical data analysis for the polyethylene production process, we designed Table 9 to store data about the equipment, craft, variable, and optimal value of the polyethylene products. Thus, Table 9 shows the structure of the product

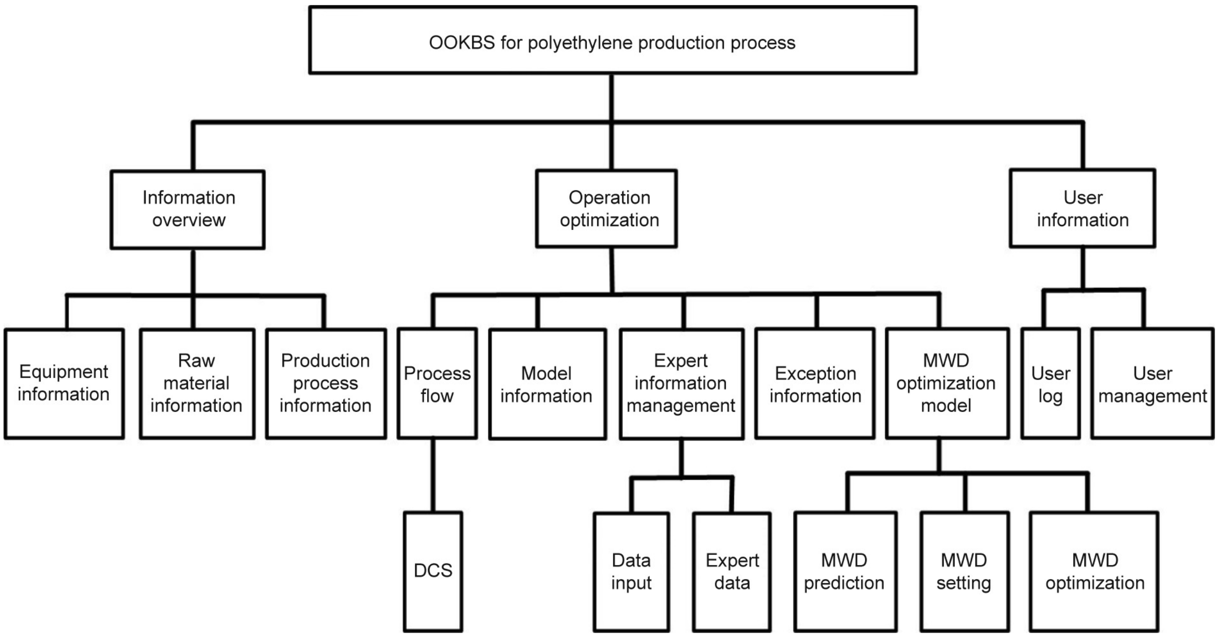

Fig. 5. Diagram of the application layer. DCS: distributed control system.

Table 9
Product information structure.

Field name	Type of field	Description
Equipment	Integer	ID of equipment
Craft	Integer	ID of craft
Variable name	Varchar (50)	Variables of polyethylene produce
Optimal value	Varchar (50)	Optimal value of polyethylene products
Hptime	Datetime	The datetime of the event

information: chemical equipment, product craft, polyethylene types, variables, and optimal conditions.

(2) Rules. In order to obtain a more effective data analysis ability, we constructed data prediction inference rules to provide computing constraints and reduce the size of the solution space, based on the correlation analysis between the design data and the actual production data from the polyethylene production process. Table 10 is designed to store the ontology reasoning rules analyzed by the Jena API, including the rule name, rule content, and rule precondition, among others. Thus, Table 10 shows the rule structure.

(3) MWD data from experts. In the polyethylene production process, in addition to equipment data, data based on expert experience plays an important role. In the prediction process, the accuracy of the MWD prediction can be improved by a correlation analysis between experts' operational experience data and the predicted value of the model; therefore, we designed Table 11 to store the expert experience-related data.

5.3. Implementation of the OOKBS

The OOKBS was developed in Java and deployed on a Tomcat server for an industrial polyethylene process.

Table 10
Rule structure.

Field name	Type of field	Description
Rule number	Varchar (20)	Series number
Rule name	Varchar (40)	Name
Rule body	Varchar (40)	Rule content
Rule head	Varchar (40)	Precondition
Rule mark	Varchar (40)	Mark of rule

Table 11
MWD data from experts.

Field name	Type of field	Description
ID	Varchar (20)	Series number
Yuce	Varchar (20)	Predicted MWD
Youhua	Varchar (20)	Optimal MWD
Qiwang	Varchar (20)	Expected MWD

Based on the polyethylene ontology information, the polyethylene process model information and process data are displayed on the page through the data access interface. Users can modify the operation parameters on the page and browse the polyethylene process information. Fig. 6 provides the process flow diagram.

The MWD optimization module includes three parts: MWD prediction, MWD setting, and MWD optimization. When the current working conditions or previously known working conditions are inputted, the BP neural network model is invoked to predict and display the MWD curve and detailed data. The MWD curve of the product based on the input working conditions is listed in the chart. The working conditions can be adjusted (Table 8) in order to observe the products' MWD conveniently.

Regarding optimization, when the dataset of the expected MWD is fed into the system, the optimization algorithm is processed and the optimized results are produced. Fig. 7 shows a comparison between the expected curve and the optimized curve, along with details of the MWD optimization.

The results of the key operation parameters for the optimized MWD and the targeted MWD are compared in Table 12. The optimized operation parameters are very close to the targeted values, which demonstrates that the system could be used to develop a new product in industry. The results of the optimization operation, based on the calculation parameters recommended by the knowledge base system and expert experience, are in good agreement with the expected results. Although this optimization parameters are not completely consistent with the targeted values, this method improves the efficiency of the MWD calculation, and produces optimized operating parameters that better match the actual polyethylene process.

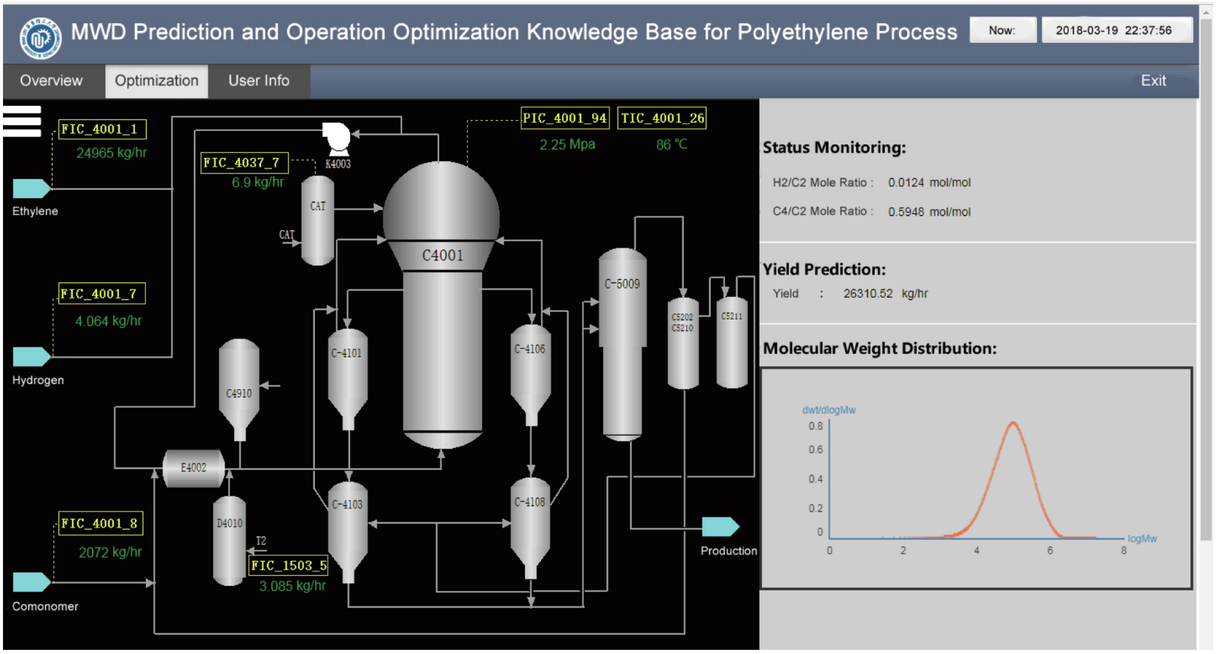

Fig. 6. Process flow diagram.

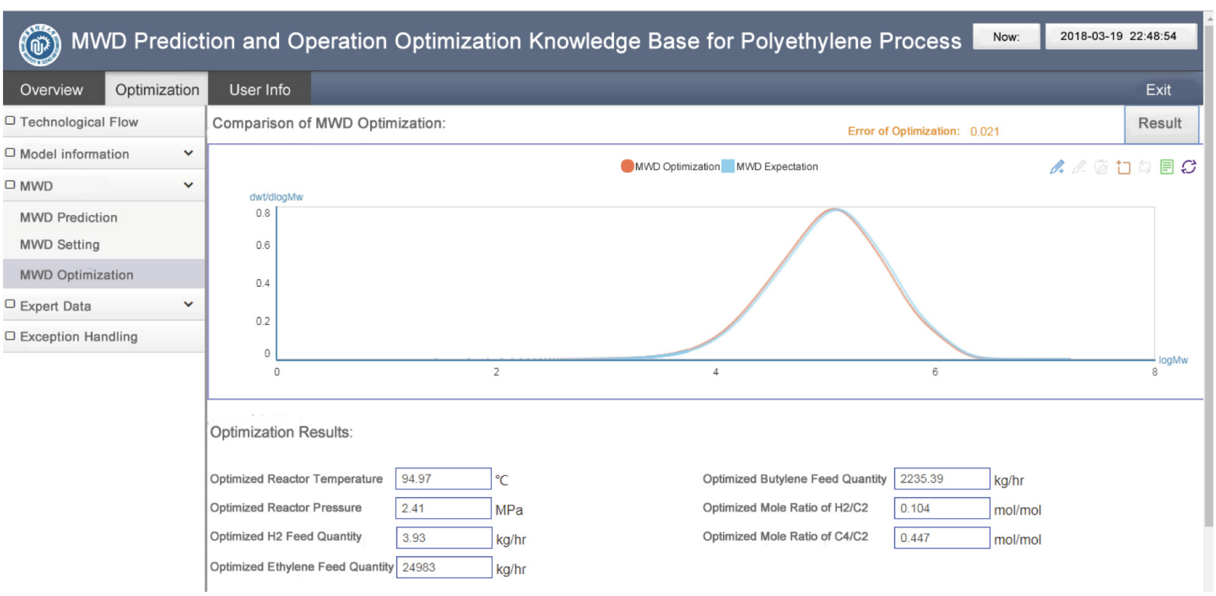

Fig. 7. A comparison between the expected curve and the optimized curve.

Table 12
A comparison of the key operation parameters for the optimized MWD and the targeted MWD.

Situation	Operation parameter						
	T (°C)	P (MPa)	$f_{C_2H_4}$	$f_{C_4H_8}$	f_{H_2}	m_{H_2}/m_{C_2}	m_{C_4}/m_{C_2}
Optimized result	94.97	2.41	24983	2235.39	3.93	0.104	0.447
Expected value	93.58	2.44	25208	2321.59	4.11	0.128	0.565

6. Conclusions

In this paper, a knowledge base system, OOKBS, designed for the operation optimization of a polyethylene process is proposed, in which an ontology is introduced to represent and share knowledge on the polyethylene process. The seven-step method is then used to construct the ontology of the polyethylene process and to unify the relevant knowledge. In the ontology library layer, the system realizes the description and storage of the ontology knowledge along with its reasoning and analysis using a Jena API, which improves the utilization ability of the knowledge base system. In the model layer, the MWD is optimized using a differential evolution algorithm, which optimizes the operating conditions. In the application layer, the system functions are designed for the operation optimization needs of the polyethylene process.

Through application to practical industrial production, the OOKBS can universally manage the process knowledge, improve the intelligence level of the polyethylene process, optimize the working conditions of the industrial process, and regulate the product structure.

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Compliance with ethics guidelines

Weimin Zhong, Chaoyuan Li, Xin Peng, Feng Wan, Xufeng An, and Zhou Tian declare that they have no conflicts of interest or financial conflicts to disclose.

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