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Study on the mode of intelligent chemical industry based on cyber-physical system and its implementation

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ABSTRACT

Responding to the technological progresses and the emerging trends of chemical industry, the mode of intelligent chemical industry based on cyber-physical system (CPS) was discussed. A structure of CPS for intelligent chemical industry was proposed, followed by the key techniques, including big data techniques and rigorous online modeling. As an example, the intelligent rectification column was elaborated. The structure of the three-agented column was proposed, to improve the optimal control level for the whole process system and promote on-line optimizing control techniques with robustness, in which CPS was the basic platform delivering the functions of surveying, communication, data storage, and computation. The optimal control models of distillation for the whole system were deduced as well; the assessment algorithms of equipment operating status, anomaly recognition, and multi-device collaboration based on the agent-oriented method were also illustrated. The operation results from the propylene rectification column showed that the intelligent rectification column proposed in the study was feasible, and met the operational requirements in terms of feedback time, stability, robustness etc.

1. Introduction

Since 1746, modern chemical industry has passed through three stages of development: the industrialization stage (chemical industry1.0), the scale stage (chemical industry 2.0), and the automation stage (chemical industry 3.0). In recent years, internet of things (IoT), big-data and artificial intelligence technologies are improving production efficiency significantly [1,2], and promoting industrial integration [3]. Specifically by combining resource, entity, man and information, the new information technology system has raised people's awareness of product innovation, diversity and product delivery speed, thus forging a new intelligent manufacturing mode [4]. Fig. 1 shows the development stages of chemical industry [5].

With the digital cyber embedding in physical system, CPS connects resource, information, physical entities and people together, integrates various computing resources, including data storage, data processing, communication, control, etc.. Based on the above properties, CPS has the capabilities of perception, communication, control and coordination, which could meet the demands of the new mode of chemical industry, so CPS could not only constitute the technical basis of multi-scale complex chemical system, but also promote supply chain integration, process optimization, and new business models. Some achievements in local applications have been gained in the applications of CPS [6–7]. Qianfeng proposed a new technology system of virtual factory based on cloud computing, by the case for an ethylene glycol virtual factory reflecting its scalability and openness [8]. R Squire established a successful cyber-physical system in the chemical industry, which achieved the automatic availability of critically needed information, thus upgraded the market response ability of enterprise [9]. But an overall architecture design and systematic research of CPS are lacked. This will make the future technology development path of chemical industry unclear, and make intelligent manufacturing mode difficult to be realized.

So this paper will propose a structure of CPS for intelligent chemical industry, and study the related techniques through a case, especial the algorithm for the complicated problems, which combines with simulation, data mining, and knowledge pieces.

Abbreviations: APC, Advanced process control; AI, Artificial intelligence; CPS, Cyber physical system; DCS, Discrete control system; ERP, Enterprise resource planning; EDI, Electronic data interchange; HSE, Health, Safety, Environment; IoT, Internet of Things; ICI, Intelligent chemical industry; MES, Manufacturing execution system; OPC, Open process control; SC, Supply chain.

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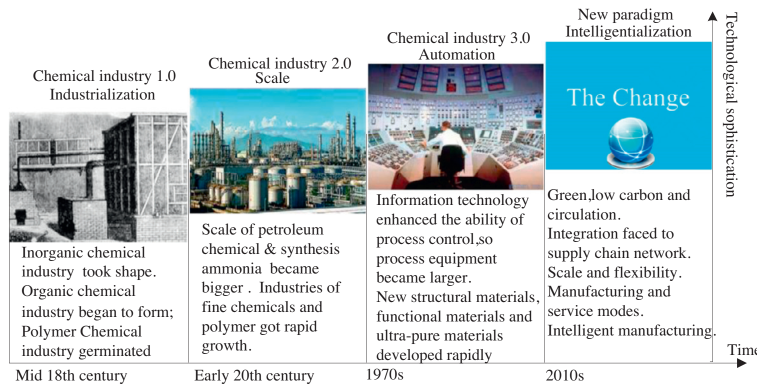

Fig. 1. The developing stages of chemical industry.

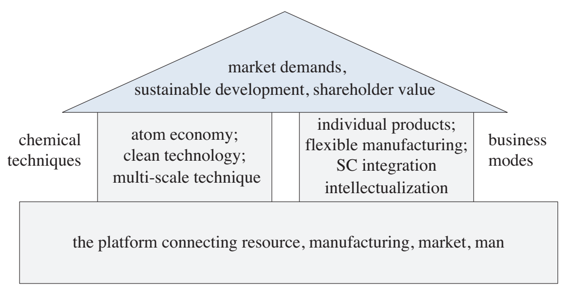

Fig. 2. The structure of intelligent chemical industry.

2. Research on the architecture of cyber-physical system for intelligent chemical industry

2.1. The mode of intelligent chemical industry

As a result of technical advances particularly the internet and IoT, a series of new industrial modes are emerging (e.g. cloud manufacturing, service-driven industry and flexible manufacturing mode [10]. Analyzing these modes, it is found that intellectualization is the common feature and even the prerequisite. As for the chemical industry, because of the specific features of its supply chain, the overall integration and optimization of the supply chain are the focuses of industrial development. [11–13]

(1) Intelligent enterprises have strong capabilities of knowledge learning and control skills, so shareholder value, market demands, and sustainable development can be integrated together.
(2) The process cooperative control mode for the whole supply chain, rather than embedded discrete control, will become the main control technique.
(3) Production organizations are transforming from “concentrated mode” characterization into as “integrated mode”
(4) With the help of comprehensive intelligence of business processes and decision-making, enterprises could adapt to more stringent environmental requirements and changing customer needs.

The framework of intelligent chemical industry (ICI) is shown in Fig. 2.

In the above structure, the chemical techniques and business modes constitute two pillars of the development of chemical industry, while the platform connecting a variety of resources is the foundation of the pillars. The comparisons between intelligent chemical industry and the conventional mode are listed in Table 1 [14]

In general, the targets of ICI are not only to improve production efficiency, but also to realize optimization of the whole supply chain. Therefore it is important to establish a strong platform for ICI that can connect the whole supply chain and have the capabilities of perception, communication, storage, computation, control, collaboration and optimization. A cyber-physical system is a good choice [15].

2.2. The architecture of cyber-physical system for intelligent chemical industry

Since the concept of CPS was proposed by NSF in 2006, many studies have been conducted on it [16]. Being a comprehensive platform on which a digital network is embedded in a physical system, CPS possesses certain autonomous ability, such as self-perception, self-judgment and self-control. Therefore it is an ideal messaging and operating platform for ICI [17]. The architecture of CPS for ICI is proposed as shown in Fig. 3. In the architecture, the cyber system connects resource, environment, production equipment and supply chain together by the aid of IoT technology, forms an exchange system of substance, energy and information facing the full life-cycle. Because CPS has much bigger multi-objective coordination capability and network integration capability than the conventional industrial control architectures, The architecture could achieve online optimization and synergy better under the background of the whole network. In addition, cloud computing platform plays an important role in the above architecture. On the basis of the real-time data of production and business, CC combining with the local computing resources solves such problems on-line or off-line as R&D, control optimization, product application, customer services, etc. The techniques applied by CC include dynamic simulation, digital simulation, knowledge management, and customization technology.

Besides perception and computation, the CPS for intelligent chemical industry emphasizes the following functional properties:

(1) Metabolism balance. Being the important mechanism to evaluate the environmental influence of material and energy flows in the manufacturing process, industrial metabolism balance is the core of future developments within the chemical industry. On CPS platform, all equipment and processes are monitored and coordinated online to make sure that resource excavation, manufacturing, consumption and waste recycling are all in equilibrium. Metabolism balance is the important assessment indicator of CPS, and also the constraint condition.
(2) Cooperative control. In order to keep the balance of material and energy inside the lifecycle of the supply chain and achieve the maximum benefits, CPS should have the abilities

Table. 1
the comparisons between the smart chemical enterprise and the conventional one.

Items	Conventional chemical industry	Intelligent chemical industry
Integration mode	Integration for processes	Integration of supply chain network
Optimization goals	Profit optimization on specific conditions	Profits optimization considering market demand, device status, energy conservation and emissions reduction.
Optimization patterns	Serial mode conducted offline	Synchronous optimization of decision-making and control adjustment employed online
Technical economic feature	Large-scale	Equilibrium between large-scale and necessary flexibility
Operation mode	Specialized manufacturing	Combination of manufacturing and service
Decision factors	Operational and technical factors	Users' requirements, products, quality standard, operating condition, resource, system reliability status.
Control mode	Discrete control	Advanced process control
Intelligent degree	Low level	Artificial intelligence embedded in the process optimization control
Control platform	Discrete control system	Contemporary integrated process system
Flexibility	Limited flexibility. adaptive scope and function redundancy	More flexible configuration. adaptive to multiple optimization control modes
Data supporting	Local small data	Big data
Algorithm	Traditional statistical analysis	Statistical analysis, data mining, AI and visualization techniques.

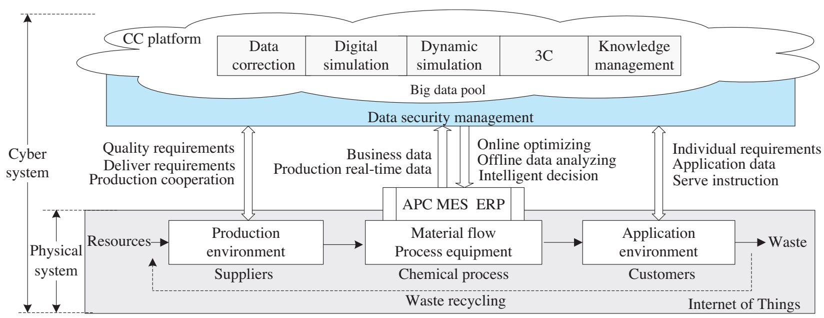

Fig. 3. The framework of the CPS for intelligent chemical industry.

of optimization, accurate control and remote collaboration for the whole supply chain.

(3) Flexibility & agility. CPS helps enterprises achieve a variety of operational objectives by means of flexible process structure, flexible configurations, lean management and fine operation. In order to maintain the balance between market and production, all enterprises in the supply chain and all operation units in the enterprise should be flexible and agile [18].

(4) Artificial intelligence (AI). Different from those in conventional control, many problems in intelligent manufacturing are unstructured, non-numerical, vague and discrete (e.g. equipment status assessment, anomaly recognition, fault treatment, process synthesis, control strategies) which are all critical for CPS's self-judgment and self-control. AI is the feasible method to enable CPS with such excellent attributes of forecast and optimization [19–21].

In order to achieve the above properties, it's important to apply big data technologies and rigorous online simulation [22].

(1) Big data technologies [23]. Big data of the chemical industry includes the data produced in management, process monitoring, planning, equipment operation and alarm information at all levels of the enterprise, which are real-time, multi-source, isomeric and dynamic. At present, the data remains underutilized, especially production real-time data and the market information data are far from reflecting its value in the integrated level. Because the CPS platform provides the basis of data collection, data marking, data processing and data-transmission, decision-making process could transfer to the active data-driven mode from the passive business-driven mode. Based on the application requirements of industrial big data, such technologies as data-collection, data preprocessing, fuzzy association and relationship model, data mining, and knowledge-oriented data warehouse, is emphasized. Certainly the small data facing to special equipment or special business is also attached importance to. In the aspect of data preprocessing, because of random errors and noisy data of real time, data is screened and corrected before transmitted to the analysis system. In order to cope with the large amount of data and the need for strict timeliness, the algorithm of distributed computing is employed, which combines local computing resources and cloud resources [24], as shown in Fig. 4. The distributed computing algorithm distributes the computational flows into different workstations according to the volume of data and the computational loads of the workstations.

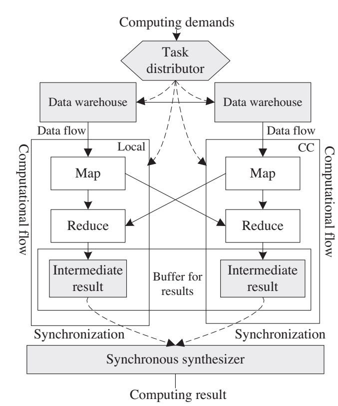

Fig. 4. The algorithm of distributed computation.

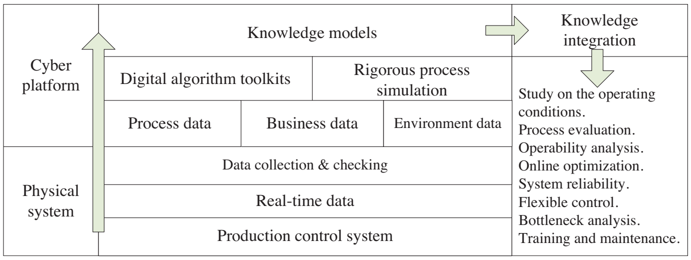

Fig. 5. The architecture of knowledge system.

(2) Knowledge system based on rigorous online modeling (ROM). ROM is a type of working condition prediction technology, combining process online simulation technology and real-time data. In the chemical industry, ROM is used to grasp the real-time operating situation and optimize the whole process system by synchronizing the digital system and the real world [25]. ROM includes offline steady-state simulation and online dynamic simulation. In the practical application, ROM requires that all models are accurate and compatible, and could conduct on-line self-learning and self-improving based on the actual operation feedback. There are some difficulties in achieving these targets. In the study, the solution with offline extraction of knowledge pieces by means of ROM and online operation support is proposed, the CPS platform being a favor basis. Namely, knowledge pieces and solutions are gained offline aiming at certain scenarios and problems by combining theoretical simulation models and gray models, and support process operation online. This is a compromise solution. Knowledge system is the crucial technical approach.

Actually, big-data technologies and ROM constitute the digital technology foundation of the knowledge system, which is the important technical approach for intellectualization, as shown in Fig. 5.

3. A case study–the smart rectification column based on CPS

Being one of the most common operation units used in the chemical industry to separate liquid mixtures into pure components, a rectification column is regulated by the preset control strategies according to the different technical parameters of the materials and the distillates [26]. The control strategies include temperature control of the stripping section, reflux ratio control, temperature difference control, recirculation flow control, etc. Because the control parameters are preset, the objective is to guarantee rectification column operation according to the default operating curve [27], rather than optimization under the dynamic condition. When a disturbance occurs such as market fluctuation, equipment performance degrades and collaborative environment among equipment change because the control configuration cannot be adjusted in real time. Continual studies on advanced control modes for rectification columns have achieved many gains, but they have been mainly concentrated on aspects of processing stability and energy conservation, with optimization mainly offline and local [28,29]. So this study will be concentrated on the online optimal control strategy facing the coordination of the whole process system based on CPS. The control models will be aimed at the overall benefit maximization and the column status predictability and controllability.

In this case study, we elaborate on a smart rectification column based on CPS. It is a test column installed in the partner factory, and is the same as the one it replaced. In operation, a mixture flow of propylene (C_3H_6) and propane (C_3H_8) is fed into

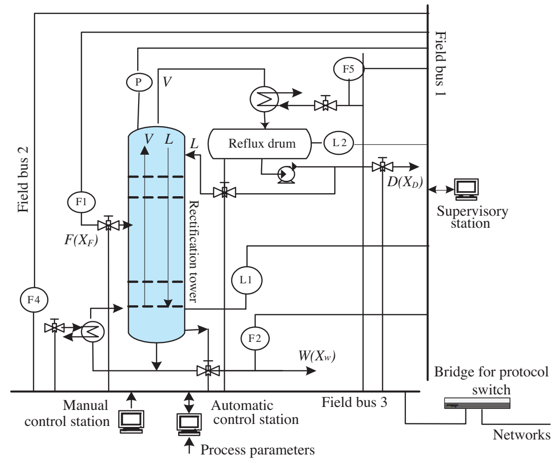

Fig. 6. The sketch map of the rectification column.

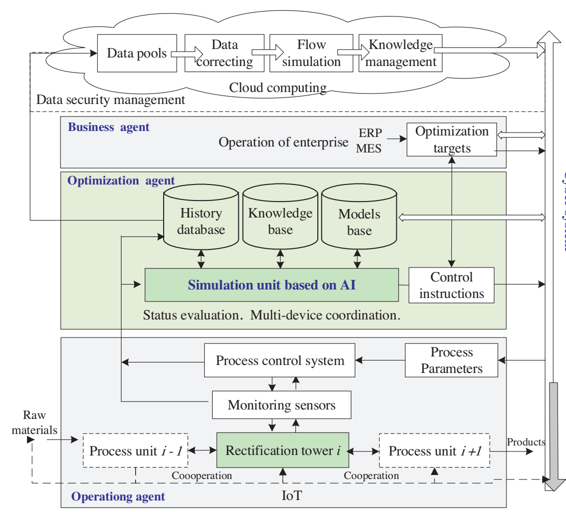

Fig. 7. The architecture of the intelligent rectification column.

the column. The product at tower-top is propylene, and propane at tower-bottom. The propylene fraction at the tower-top is required $> 99.6\%$, and that at the tower-bottom is $< 6\%$. The technical and the related economic indexes of the rectification column are shown in Table 2. The sketch map of the column is shown in Fig. 6.

In practical operation, factors such as equipment configuration parameters, feed ingredients, product types, as well as the price of products and materials, often change and lead to fluctuating operational benefits. In the conventional control mode, the process adjustment is done offline, and is completed often in one week starting with the next production cycle. In order to enhance the ability of the rectification column to address different situations, a smart rectification column is established based on CPS. As shown in Fig. 7, the whole rectifying column system based on CPS contains three agents: a business agent, an optimization agent and an operation agent. Through the cyber system, the rectification column could connect computing units, business units and optimization units.

To achieve intelligent operation, there are there key functions that need to be addressed: the optimal control model of the rectification column, the flexibility of the rectification column, and the operability and robustness of the model under the condition of industrial control.

Table 2
Operating criterion for propylene rectification column.

Items	Feed	Component of the feed%		Propylene	Propane	Reflux rate	Energy wastage	Feed profit rate
		Propylene	Propylene					
Flow rate(kmole.s^{-1})	21.50	93.50	5.12	18.14	1.86	18.5	79.7	
Price(yuan.t^{-1})	3250.00			7300.00	4150.00		81.00	2.03

Note: Energy wastage denoted by stream quantities.

3.1. The optimal control model of the rectification column

According to the relationships of the inflows and outflows shown in Fig. 6 and the actual production requirements, the flow rate of feed, component, vapor flow rate, and products' prices are set as the influencing factors; reflux ratio, tower-top distillate flow rate, and tower-bottom distillate flow rate as control parameters; and optimal economic profit as the goal of the control strategy [30]. Considering the column operation fee, the raw materials cost, and the value of the distillates, the maximization of the net income of the rectification column is selected as the optimal control objective function, being expressed as:

$$\max P^{\Delta t} = income_{top}^{\Delta t} + income_{bottom}^{\Delta t} - cost_{raw}^{\Delta t} - cost_{energy}^{\Delta t} - cost_{fee}^{\Delta t}$$

Namely, the operating net income equals the income of the tower-top distillate plus that of the tower-bottom distillate, minus the raw material cost, the energy cost, and the column operating fee. The superscript "Δt" presents the values in the "Δt" time interval. Therefore calculating the profit in the operating period "T", it could be expressed as the formula (1).

$$MaxP = \int_0^{\mathrm{T}} (p_1^t \cdot D^t \cdot X_D^t + p_2^t \cdot W^t \cdot (1 - X_w^t) - C_1^t \cdot F^t - C_H^t \cdot H_\nu \cdot V^t - C_F^t)dt \tag{1}$$

Where "P" represents the operation profit, "p_1^t" the propylene price, "p_2^t" the propane price, "C_1^t" the cost of the feeding liquid, "C_H^t" the vapor cost; "F^t" the feeding flow rate (Kmol.S^{-1}), "D^t" the tower-top distillate flow rate (Kmol.S^{-1}),"W^t" the tower-bottom distillate flow rate (Kmol.S^{-1}), "X_F^t" the mole fraction of propylene of the feeding flow, "X_D^t" the mole fraction of propylene of the tower-top distillate, "X_W^t" the mole fraction of propylene of the tower-bottom distillate, "H_v" the latent heat of vaporization of the feeding liquid (KJ.Kmol^{-1}), "V^t" the vapor rate (Kmol.s^{-1}), and "C_F^t" the operation fee. The superscript "t" presents the values at the time t.

According to the operation models of distillation, there are relationships between the variables in formula (1). These models constitute the ROM of the rectification column, mainly including material balance models and energy balance models, as shown in formula (2–5):

Material balance:

$$F^t + V^t = W^t + D^t \tag{2}$$

$$V^t = (R^t + 1)D^t \tag{3}$$

$$F^t \cdot X_F^t = W^t \cdot X_D^t + D^t \cdot X_D^t \tag{4}$$

Energy balance:

$$K \cdot Ln\left(\frac{X_D^t(1 - X_w^t)}{X_W^t(1 - X_D^t)}\right) = \frac{V^t}{F^t} \tag{5}$$

where "K " is the feature factor of the column, which is decided by the tray type and the packing type of the column "R^t" the reflux rate.

The rectifying column optimal operation also has constraint conditions. For instance, the amount and type of distillates should meet the requirements of those units before and after distillation, the contract quantity, and the minimum load requirement of the column. The constraint conditions are shown in formula (6,7).

$$\int_0^{\mathrm{T}} \left(D^t \cdot X_D^t\right)dt \geq D_c \tag{6}$$

$$R_f^t \geq R_{f\,\min}(R_f^t = M_f^t \cdot B_s^t) \tag{7}$$

Where "D_c" is the contract order quantity or the minimum process material flow, "R_f^t " is the function reliability,"M_f^t" is the operating rate,"D_s^t" is the load rate, "R_{fmin}" is the minimum function reliability, and "T" is the working period.

It can be found that the above optimal control models are a combination of the integral model and the instantaneous rigorous simulation models. While actually calculating, a grid algorithm based on time dimension is applied. For example, formula (1) is converted as:

$$\max P = \sum_{\Delta t=0}^{T} (\bar{p}_1^{\Delta t} \cdot D^{\Delta t} \cdot \bar{X}_D^{\Delta t} + \bar{p}_2^{\Delta t} \cdot W^{\Delta t} \cdot (1 - \bar{X}_w^{\Delta t}) - \bar{C}_1^{\Delta t} \cdot F^{\Delta t} - \bar{C}_H^{\Delta t} \cdot H_\nu \cdot V^{\Delta t} - C_F^{\Delta t}) \tag{8}$$

Where "$\bar{p}_1^{\Delta t}$" is the average propylene price in the "Δt" time interval; "$D^{\Delta t}$" is the total flow at the tower-top in the "Δt" time interval (Kmol); and so on.

While searching optimization, the deviation between the calculated values and the real operating data are analyzed continually according to the formula (8). The smaller the oscillation deviation, the higher is the degree of control optimization. But if the target deviation is too small, the robustness of operation control would be reduced, and the stability of rectifying operation would also be reduced.

$$\sum_i^N \sum_t^M (\chi_{i,t}^d - \chi_{i,t}^c)^2 \leq \xi \tag{9}$$

Where, "$\chi_{i,t}^d$" is the real-time data of variable "i" collected at time "t". "$\chi_{i,t}^c$" is the analog data of variable "i" at time "t", and "ξ" is the target deviation between the calculated values and the real operating data. In actual operating, the business data are collected from the ERP, and the equipment operating status data and processing data are collected from DCS.

3.2. The flexibility of the rectification column

In order to adapt to the different situation, the rectification column should be flexible [31]. The steady state of the rectification column is described as the follows:

$$h(d, z, \chi, \theta) = 0 \tag{10}$$

$$g(d, z, \chi, \theta) \leq 0 \tag{11}$$

where: h is the equality constraints, including formula (2–5); g is the inequality constraints including formula *(6,7); d* is the vector *of* design variables which keep fixed during the operation; vector χ is the state variables(e.g. C_F,C_H, V, X_F,X_D, X_W, H_v, K, F, *etc.*); vector z is the control variables(e.g. *D, W, R, etc.*), namely the degree of operation freedom; vector θ denote the unpredictable factors, which

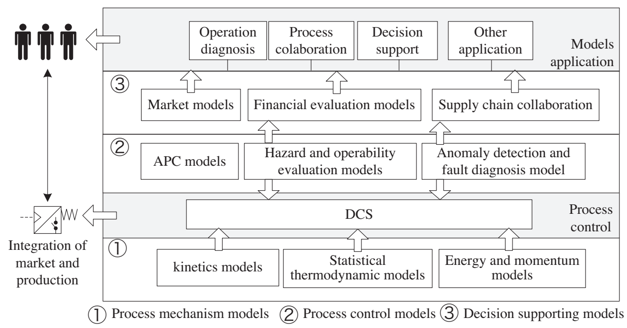

Fig. 8. Three-layer process simulation models.

include either internal process influencing parameter or external influencing parameters(e.g.p_1, p_2, C_1,R_f, M_f, D_s,*etc.*).

By eliminating vector χ, the above formulas could be simplified as follows:

$$\chi = \chi(d, z, \theta) \tag{12}$$

$$f(d, z, \theta) \le 0 \tag{13}$$

To build the models of flexible operation, the uncertain conditions in actual operation are taken into account. The operation-feasible values range of θ decides the size of flexible region of rectification tower. Hyper-rectangle is used to describe the range of θ. Setting the nominal point θ^N, two corresponding positive and negative deviations$\Delta\theta^+$,$\Delta\theta^-$ and the scalar parameter δ, so the range of θ is

$$T(\delta) = \{\theta | \theta^N - \delta\Delta\theta^- \le \theta \le \theta^N + \delta\Delta\theta^+\} \tag{14}$$

For formula (14), δ is the key index, and mainly based on experience. From the above formula, the hyper-rectangle determines the actual size of the region for feasible operation under uncertain conditions. In conventional rectification process, the adjustment strategy of z is to meet the requirement of nearly fixed range of hyper-rectangle, only considering the device itself, called "local adjusting method". Now based on CPS, the coordination of multi-devices and multi-processes ask bigger range of θ and Z. For the range of θ being as large as possible, the constraint conditions are expressed as

$$\max_{\theta\in T(\delta)} \min_{z} \max_{i\in I} f_i(d, z, \theta) \le 0 \tag{15}$$

$$T(\delta) = \{\theta | \theta_i^N - \delta_i\Delta\theta_i^- \le \theta_i \le \theta_i^N + \delta_i\Delta\theta_i^+\} \tag{16}$$

Where: i presents the correlation process i, I is the set of all correlation processes, which could be process units, business operation, or decision-making. The new mode is called "coordination adjusting method". Establishing the set I is the critical procedure for "coordination adjusting method", so the process coordination models are expanded as shown in Fig. 8, which contains three-layer.

3.3. The operability and robustness of the optimal model under the condition of industrial control

Because of the spatial-temporal interaction of the control system and the equipments, as well as the non-determinism of the operation environment (e.g. the set I likely changes under different condition), the above optimal control models could not satisfy the every actual operational demands. As the dynamic optimal control is a non-stationary coupling process varying with time, it is different from the conventional column. The decision variables have the characteristics of time variation, randomness, correlation and dynamics, so the robustness and anti-interference of intelligent control are very important. This involves some unstructured problems, such as equipment operating status evaluation, anomaly recognition, multi-device coordination and the like. The algorithms dealing with those unstructured problems are critical [32]. The algorithms based on the knowledge base could be feasible methods. The key elements to be resolved are extraction and release of the rules [33]. Fig. 9 illustrates three specific algorithms of the unstructured problems based on knowledge base.

The agent-oriented method for the above unstructured problems is studied. According to the control features of rectification column, the agent-oriented classes are classified as object class (OC) and agent class (AC). OC is the structural description of the equipment configuration information and the actual operating data according to certain rules. OC connects the real-time database and the history database online. The object class (17) is an example of the column monitoring

Class column_detect
{ string t —*the monitor time*
float F; —*the real – time feeding flow rate*
float W; —*the real – time tower – bottom distillate flow rate*
float D; — *the real – time tower – top distillate flow rate*
float V; —*the real – time vapor rate flowing into the reboiler*
float R; —*the reflux rate of the reflux drum* (17)
float p_1; —*the price of product*
float p_2 —*the cost of raw material*
float c_1 —*the operating fee of the equipment*
. . . . . .
}

AC describes the field knowledge (e.g. anomaly recognition and operating status judgment). Knowledge pieces are created by associating diverse AC through a reasoning process or rules. Segment (18) is the fundamental form for the knowledge pieces of the rectification column which encapsulates the related knowledge of distillation process control. The object class "*column_detect*" and "*decision_scope*" denote the corresponding operating data and the constraint condition

Segment control_solution : public solution
{ column_control data_control; —*optimal operating strategies from knowledge base*
column_detect data_detect; —*the corresponding operating data*
decision_scope constrant_inf; —*the constraint condition*
product product_inf; —*the information of products*
resource resource_inf; —*the information of raw materials*
others other_inf; —*the related information (e.g. environmental condition, financial information, etc.)*
}
(18)

class decision_scope
{ material balance; —*the models of material (energy) balance*
market market_inf; —*the market information*
requirement requirement_inf; —*the customer requirement information*
sale sale_inf; —*the information of contract and production scheduling*
power power_inf; —*the consumption of energy*
equipment equipment_inf; —*the equipment operating status*
}
(19)

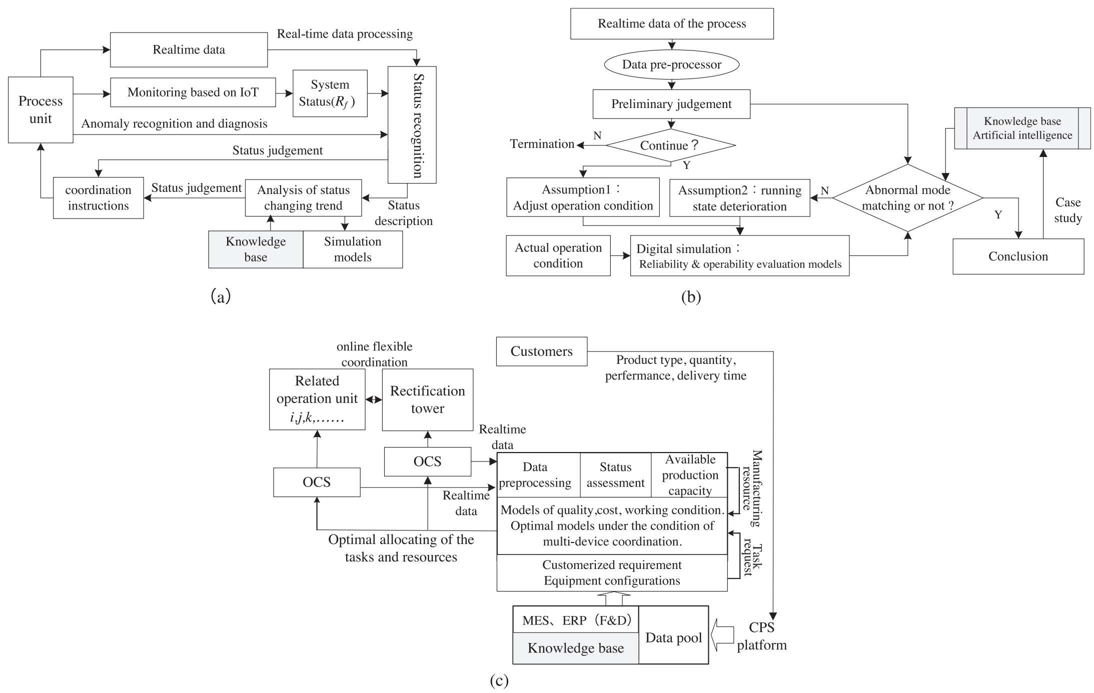

Fig. 9. The algorithms of unstructured problems based on knowledge base (a) The assessment algorithm of equipment operating status evaluation; (b) The algorithm of anomaly recognition; (c) The algorithm of multi-device coordination for rectification column.

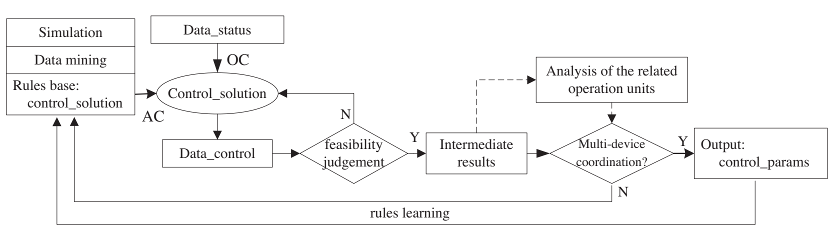

Fig. 10. The algorithm of automated reasoning based on knowledge base.

The computational procedures of importing OC into AC and outputting the corresponding conclusions are called automated reasoning, through which the process data of distillation and the operating status of the rectification column match the optimal operating strategies in the knowledge base. Besides the optimal control strategies under complex conditions, equipment operating status evaluation and anomaly recognition could also be addressed by means of automated reasoning. Inference (20) shows the automated reasoning of the "*control_solution*"

$$\begin{aligned}
&\text{Inference Control_solution}\\
&\quad \text{Roles :}\\
&\qquad \text{input : data_status;}\\
&\qquad \text{output : control_params;}\\
&\qquad \text{method : control_solution;}\\
&\qquad\qquad \text{simulation;}\\
&\qquad\qquad \text{data mining;}\\
&\quad \text{Specification :}\\
&\qquad \textit{"Each time the inference is invoked, it generates}\\
&\quad \textit{a candidate solution that could change the}\\
&\textit{operation conditions of the associated units."}\\
&\text{End inference control_solution}
\end{aligned} \tag{20}$$

The algorithm of automated reasoning is shown in Fig. 10.

When operating, the simulation unit of the optimization agent gets real data from multi-data sources; then it executes process simulation, process status evaluation, and collaborative inspection of the relevant units; and finally it makes optimal decisions and control schemes. The algorithm of the optimal decision-making is shown in Fig. 11.

3.4. The realization of smart control

To realize smart control, the online control system should collect various local signals, read the environment information from the other systems efficiently, and finish complex computation. Obviously the conventional DCS could not meet the requirements. So the embedded control system facing complex tasks based on ARM chip are developed. Fig. 12 is the control board which uses ARM chip as processor and could deal with analog signal and digital signal simultaneously, integrate Ethernet interface and CAN interface, connect with ERP, MES, and LIMS, and undertake complicated computing. Thus a 4-level architecture of distributed computation resources is formed, composed of node resources (ARM), local control resources (online control system), enterprise-scale resources and cloud computation resources. The computation demands are distributed according to the requirement of time effectiveness as well as the scope of data integration. Those computation demands which are based on the definite knowledge rules and have strong timeliness requirement are executed by ARM instantly, e.g. equipment operating status evaluation and anomaly recognition. The information integration of ERP\MES\LIMS, decision making, and the compilation of control instructions are finished by the enterprise local resources. While those computations required comprehensive data integration mainly based on historical data, such as data

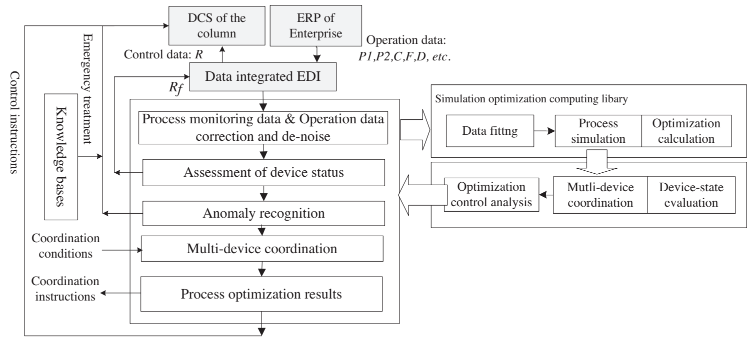

Fig. 11. The algorithm of optimal decision-making.

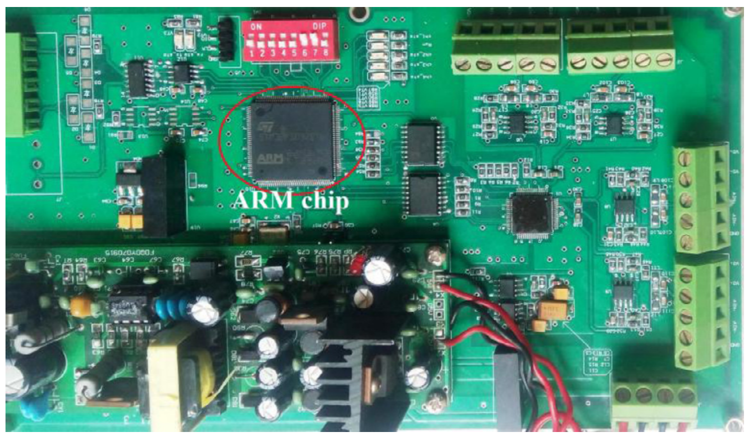

Fig. 12. The control board with ARM chip being core processor.

Table 3
The optimal results of the rectification column after some conditions changing.

Changing items	Changed value	Reflux rate	Tower-top propylene	Tower-bottom propylene	Energy wastage	Feed profit rate	Feedback time/(Min)
Feed /kg.s^{-1}	24.5	18.5	99.63	4.9	86.5	2.08	3.87
Component changing	C_3H_6:92.3; C_3H_8:6.3	19.2	99.61	5.5	82.3	2.04	4.12
Heat from reboiler /KJ	Reduce 5%	26.2	99.60	5.7	92.3	1.96	4.35
Cooling water in reflux drum /m^3.s^{-1}	Reduce 5%	23.7	99.60	5.9	91.5	1.98	4.55
Stream price /yuan.m^{-3}	185	18.3	99.60	5.2	80.5	2.03	3.85

mining, rule educing, decision model improving, etc., are executed by CC and the other computation resources cooperatively. For example, in the computation process of improving equipment status evaluation models, CC finishes mining historical data and analyzing the model, synchronously the ARM verifies the boundary of the model and tests its correctness. So by means of the distributed computation system built on the CPS platform, the process control and the system coordination evaluation are executed synchronously at the equipment scene, ensuring the performances of intelligent control, the control strategies and evaluation models are constantly updated according to the changes of production environment and operation requirements.

In the practical operation of CPS, equipment, materials, products, environment and market are monitored online, production real-time data, supply-chain data, business environment data are gathered, corrected, related, and mined, also process control optimization, abnormity diagnosis, production scheduling, and managing decision are performed under the conditions of multi scenario and multi objection. In the rectification column case, the reflux rate(R) is adjusted automatically at a fixed period to achieve optimal economic profit along with the changes of operating conditions by means of the aforesaid models and algorithms. Some actual optimal results in diverse conditions are listed in Table 3, which shows that the feed profit rates are almost larger than 2.03. The lower profit rates (e.g. 1.96, 1.98) are because of the bigger cost of steam or the presence of tougher conditions. All feedback times are < 5 minutes.

The results prove that the smart rectification column could meet the operating requirements in terms of operation benefits, product quality & output, feedback time, stability, and robustness. In particular, alignment and collaboration between several units is improved significantly. Despite all this, considering the complex of chemical process and the rigid requirements for the robustness, stability, and reliability, we think more and lager scale case studies are necessary to confirm the applicability of the CPS architecture.

4. Conclusions

This article analyzed a mode of intelligent chemical industry, proposed a framework of a cyber-physical system as the basic platform for the mode based on the characteristics of chemical industry and embodying the requirements of the industry development. The key techniques of CPS were also studied, including big data techniques and knowledge system based on rigorous online modeling. As a case, an intelligent rectification column was explored, which could meet the column's operational requirements in terms of feedback time, stability, robustness, etc. Following were the main achievements:

(1) Aiming for online optimization, the structure of intelligent rectification column based on CPS was established, characterized by three-agent structure, multi process integration, and online optimization, which contained almost all the basic elements of chemical unit operations except chemical reaction, and therefore had a certain general significance. But different chemical unit operation had different timeliness requirements, different requirements for stable control, and different requirements for reliability assurance. This was why the intellectualization of chemical industry was much more difficult than that of discrete industries. So the applicability and performance of the proposed structure need continuously improving.
(2) Comprehensively considering the column properties, the constraint conditions, and the objective functions for optimization, the control models of distillation were deduced combining with the rigorous online modeling and the knowledge models based on big-data techniques. The CPS platform provided the foundation for the algorithm of optimal decision-making facing the collaboration between multi devices. For chemical industry, multi device cooperative control based on CPS platform is the basic requirement of intelligent manufacturing and also the important characteristics differing from the conventional advanced control.
(3) The algorithms of unstructured problems based on knowledge base were studied in order to improve operability and robustness of the system. The agent-oriented method was illustrated as the foundation of the assessment algorithm for equipment operating status evaluation, anomaly recognition, and multi-device collaboration. The algorithm of automated reasoning combining with simulation, data mining, and knowledge pieces was expected to solve those unstructured problems, and was probably among the most helpful methods for solving complicated problems.

Clearly, whether the smart rectification column based on CPS could be applied in a greater scope depends on the efficiency of real-time data processing, the accuracy of the models facing a variety of situations and the network security. So did the structure of intelligent chemical industry and the online optimal control methods. In addition, the proposed monitoring techniques based on IoT, and the dynamic simulation techniques based on big data need further research, both the sensitivity and robustness of the column control are also worthy of further work, noting that these, which are the key evaluation criteria of online optimal control.

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Reference

[1] Heiner L, Peter F, Hans-Georg K, DIT F, DHM Hoffmann. Industry 4.0. Bus Inf Syst Eng 2014;6:239–42.
[2] Posada J, Toro C, Barandiaran I, Oyarzun D, Stricker D, Amicis R, et al. Visual computing as a key enabling technology for industrie 4.0 and industrial internet. IEEE Comput Graphics Appl 2015;35:26–40.
[3] Yang YQ, Jiang XY. Development strategy of China's chemical industries if merge of industrialization and information. Mod Chem Ind 2009;29:9–13.
[4] Alexander V, Armin L, Jan S. Globalized cyber physical production systems. Prod Eng 2013;6:643–9.
[5] Cussler EL, Moggridge GD. Changing chemical industry. Rev Chem Eng 2012;28:73–9.
[6] Jay L, Hung AK. Service innovation and smart analytics for Industry 4.0 and big data environment Procedia. CIRP 2014;16:3–8.
[7] Tao F, Zuo Y, Xu L. Zhang L IoT-based intelligent perception and access of manufacturing resource toward cloud manufacturing. IEEE Trans Ind Inf 2014;10:1547–57.
[8] Luo N, Wan F, Ye ZC, Du WL, Qi RB, Zhong WM, Qian F. Cloud computing and virtual reality based virtual factory of chemical processes. Chem Ind Eng Progress 2012;31(12):2815–19.
[9] Squire R, Song H. Cyber-physical systems opportunities in the chemical industry: a security and emergency management example. Process Safety Progress 2014;33(4):329–32.
[10] Damir H, Alojzij S. A conceptual framework for a ubiquitous autonomous work system in the Engineer- To-Order environment. Int J Adv Manuf Technol 2015;78:1971–88.
[11] Lin Z, Luo YL, Tao F, Li BH, Ren L, Zhang XS, et al. Cloud manufacturing: a new manufacturing paradigm. Enterprise Inf Syst 2014;8:167–87.
[12] Chen XD, Fu WQ, Zhou H, Chen Y. The applications and trends of the next generation network technology in petroleum and petrochemical industry. Comput Appl Chem 2013;30:912–16.
[13] Li DF, Suo HS. Accelerate the process of smart plant, promote ecological civilization construction. CIESC J 2014;65:374–80.
[14] Ji X, Zhu LJ, Zhao F, Tang JH. Research on knowledge modelling system oriented to knowledge management for process enterprises. Comput Integrated Manuf Syst 2006;3:382–9.
[15] Zhang LC. Convergence of physical system and cyber system modeling methods for aviation cyber physical control system. In: Information and Automation (ICIA), 2014, 6. IEEE; 2014. p. 542–7.
[16] Khaitan SK, McCalley JD. Design techniques and applications of cyber-physical systems: a survey. IEEE Sys J 2015;9:350–65.
[17] Leonard B, Makoto T, Farookh KH. Special issue on emerging trends in cyber–physical systems. J Ambient Intell Humanized Comput 2011;2:249–55.
[18] Hong SP, Ngoc HT. An autonomous manufacturing system for adapting to disturbances. Int J Adv Manuf Technol 2011;56:1159–65.
[19] Yuan Z, Wang L-N, Ji X. Prediction of concrete compressive strength: research on hybrid models genetic based algorithms and ANFIS. Adv Eng Softw 2014;67:156–63.
[20] Ngai EWT, Li C-L, Cheng TCE, Venus Lun YH, Lai K-H, Cao J. Design and development of an intelligent context-aware decision support system for real-time monitoring of container terminal operations. Int J Prod Res 2011;49:3501–26.
[21] Bhalla D, Bansal RK, Gupta HO. Integrating AI based DGA fault diagnosis using Dempster-Shafer theory. Int J Electric Power Energy Syst. 2013;48:31–8.
[22] Lluvia M, Ochoa E, Megan J, Robin S. Operational optimization of crude oil distillation systems using artificial neural networks. Comput Chem Eng 2013;59:178–85.
[23] Hashem IAT, Yaqoob L, Anuar NB, Mokhtar S, Gani A, Khan SU. The rise of "big data" on cloud computing: review and open research issues. Inform Syst 2015;47:98–115.
[24] Bogdanova VG, Bychkov IV, Korsukov AS, Oparin GA, Feoktistov AG. Multiagent approach to controlling distributed computing in a cluster Grid system. J Comput Syst Sci Int 2014;53:713–22.
[25] Chen K, Tian Z, Luo N, Liu B. Modeling and simulation of borstar bimodal polyethylene process based on a rigorous PC-SAFT equation of state model. Ind Eng Chem Res 2014;53:19905–15.
[26] José AC, Ignacio EG. Optimal synthesis of thermally coupled distillation sequences using a novel MILP approach. Comput Chem Eng 2014;61:118–35.
[27] Li GZ, Bai P. New operation strategy for separation of ethanol–water by extractive distillation. Ind Eng Chem Res 2012;51:2723–9.
[28] Mirko S, Andreas H, Wolfgang M. Efficient optimization-based design for the separation of heterogeneous azeotropic mixtures. Comput Chem Eng 2015;72:34–51.
[29] Carlo ET, Massimiliano E, Ben-Guang R. Design and optimization of modified non-sharp column configurations for quaternary distillations. Comput Chem Eng 2015;74:15–27.
[30] El-Tamimi AM, Abidi MH, Mian SH, Aalam J. Analysis of performance measures of flexible manufacturing system. J King Saud Univ–Eng Sci 2012;24:115–29.
[31] Luyben WL. Design and control of a fully heat-integrated pressure-swing azeotropic distillation system. Ind Eng Chem Res 2008;47:2681–95.
[32] Aradhye HB, Bakshi BR, Davis JF. Clustering in wavelet domain: a multiresolution ART network for anomaly detection. AICHE J 2004;50:2455–66.
[33] Mazinan AH, Sheikhan M. On the practice of artificial intelligence based predictive control scheme: a case study. Appl Int 2012;36:178–89.