DESIGN OF A NEW IPC-MODE CHEMICAL PROCESS OPERATOR-TRAINING SIMULATOR

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Abstract

The design of an operator-training computer simulator for chemical processes is very important in the process control and simulation area. In this paper, an operator-training simulator is developed for a small-scale fine chemical production process using an IPC (industrial personal computer and intelligent process controller) simulation mode and a typical SCADA (supervisory control and data acquisition) configuration software as the GUI (graphical user interface) platform. The dynamic behavior of the process is modelled by the dynamic compensation modelling method. The overall simulation software package is successfully integrated by the designed DLL (dynamic link library) function program, which is used to link the dynamic model calculation program to the simulation GUI through the database of the SCADA configuration software. The simulator is demonstrated to have good performance in chemical process operator-training practice.

1 Introduction

In recent years, it is very common to use a simulator to train chemical process operators in advanced chemical process industry as this makes operation training more vividly and efficiently [2, 5, 7, 12, and 13].

Traditionally, the development of process simulation systems is concentrated on operator-training simulators for large-scale continuous running petrochemical and chemical processes. Until now, the operator-training simulators for fine chemical production processes, especially for small-scale processes, have very little research [1, 12].

The fine chemical production processes are usually small-scale batch or semi-continuous production processes with long and complex flow sheets, strong corrosion chemicals and frequent changing process characteristics. So their operation and control is quite complex. But fine chemical products generally have high economic benefit due to low cost, high profit and great demand market. So their production gradually attracts more and more attention. Using real processes to train process operators for fine and special chemical production processes has many limitations due to its complex technique requirements. So using a computer simulation system to train operators is largely needed in this area [1].

In general, DCS (distributed control system) simulators are used to train operators in large and medium scale chemical processes. However, in small-scale chemical processes, the situation is different. Because most small-scale chemical processes are monitored and controlled by industrial personal computers (IPC) or intelligent process controllers (IPC) using standard configuration software for SCADA (supervisory control and data acquisition) systems [4,8]. So, in this paper, a new kind of computer simulators for the small-scale chemical process operation training is developed, based on a personal computer (PC) and configuration software, which is called the new IPC-mode simulator.

The IPC-mode process simulator [11] can run on personal computers, whose cost is very low. In the IPC-mode simulator, the GUI, training teacher's functions and dynamic simulation models are integrated into one package. It can simulate the whole process of a medium-scale or a small-scale chemical process or a production unit. The simulation training functions of the IPC-mode simulator are also powerful.

Wu [11] introduced the concept of IPC-mode operator-training simulator and also developed several simulation software packages for some typical chemical engineering operation units. As the GUI of the packages was programmed in C rather than by the standard SCADA configuration software, the development of the GUI is not flexible. In addition, the program for the calculation of process simulation models was also completed using C and mixed with the GUI software, which is not integrated with a dynamic link library. The software for the GUI and the calculation of process simulation models was hard to be modularized. Thus, the IPC-mode simulator development method in [11] is too complicated for chemical engineers and control engineers to use.

In this paper, a novel and convenient design method is developed for the IPC-mode process simulator. The main scheme for the design of the IPC-mode training simulator's software is as follows: The configuration software is used as a platform to develop the simulator's HMI (human machine interface). The HMI receives operator's commands and displays simulated results of the process model by the

designed process flow sheets and simulation training command buttons. The dynamic behavior of chemical processes is modelled using the dynamic compensation method. The exchange of dynamic data in the database between the configuration software and the process model is conducted by a dynamic link library (DLL) function.

The new IPC-mode training simulator is applied to the operator-training of a real small-scale chemical process – 06 production process. The application results show that the simulator is reliable, accurate and vivid for the operation training. They also illustrate that the IPC-mode simulator is suitable for the operation-training of small-scale chemical processes.

2 Main Scheme and Principle

As an IPC-mode simulator, the hardware of the simulator can be a personal computer (PC) or an industrial PC. So the main work of the small-scale chemical process operator-training simulator concentrates on the design of the simulation software. The main structure for the design of the IPC-mode training simulator's software is given in Figure 1.

A commonly used configuration software for industrial automatic monitoring and control, CENTURY STAR [3], is used as the platform to develop the simulator's GUI. The CENTURY STAR possesses comprehensive human machine interface (HMI) developing ability, powerful SCADA functions and fully customizable graphs displaying and charting utilities. The GUI of the new IPC-mode simulator can be created, relying on the powerful color graphs plotting, process parameters dynamic displaying, command buttons manipulation, dynamic parameter input and output, and command language programming functions of the CENTURY STAR.

The dynamic models of the small-scale fine chemical process are built by the dynamic compensation method. The calculation software of these dynamic models is programmed using Visual C++ (VC++), then a dynamic link library (DLL) program UserFunc.dll is created by compiling the VC++ program. UserFunc.dll is used to dynamically link the database of CENTURY STAR and the dynamic process models.

During the training, operators can enter their operation instructions to the SCADA configuration software CENTURY STAR by clicking on the command buttons and icons of process equipments in the simulation flow sheets. CENTURY STAR will store these operation instructions into its database and transfer them to the dynamic models to do calculations through UserFunc.dll. The calculation results of the models will be transferred and stored into the database of CENTURY STAR by UserFunc.dll and displayed in the simulation flow sheets of CENTURY STAR. At the end, a comprehensive operator-training simulator can be built by adding some simulation command buttons such as ACCIDENT SETTING, TIME-SCALE SETTING, SNAPSHOT SETTING and SCORE EVALUATION etc. into the simulation flow sheets of CENTURY STAR.
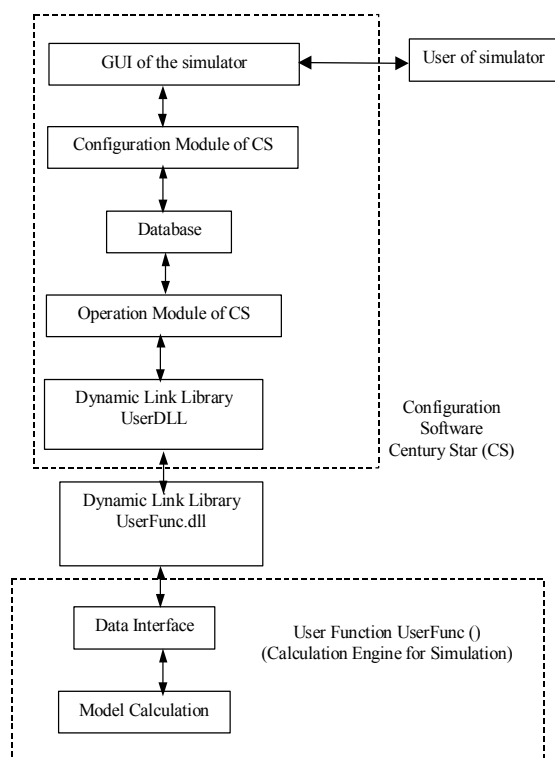

Figure 1: Main structure of the new IPC-mode training simulator's software

3 Building Process Models

06 production process is composed of three sectors: reaction of 01 and 02 to produce the intermediate material 03; reaction of 03 and 04, and depickling to produce raw 06; distillation by adding 05 and refining of raw 06 to achieve the final product - fine 06.

3.1 General Description of Building Process Models

The process models are built in the following steps.

Step 1: Build process models either by theoretical analysis methods (including mass balance, energy balance and reaction kinetics of the process) or by system identification and parameter estimation methods (using process data).

Step 2: Simplify and discretize the process models.

Step 3: Transform process static models into dynamic models using the dynamic compensation method to obtain process simulation models.

Step 4: Carry out verification, validation and accreditation (VV&A) test of the process simulation models.

Step 5: If the process models satisfy the simulation requirements, the procedure of building process models terminates. Otherwise, repeat the modeling cycle from Step 1.

In terms of the production process of 06 and its simulation requirements, the whole process model consists of 7 parts:

Part 1: Basic physical and chemical property models of the process materials.
Part 2: The models of key production equipment, including reactors, distillators, heat exchangers, centrifuges and et al.
Part 3: The models of process interlock and alarm systems.
Part 4: The models of process accidents.
Part 5: The models of simulation training functions of the process simulator.
Part 6: The models of sound and animation of the simulator's GUI.
Part 7: The models of automatic controllers, valves, pipelines and other supplement models.

Some typical models like the reaction models of 03 production, the model of assessing operators' performance based on their operation record of the process simulator, and the key modeling method – the dynamic compensation method will be discussed below.

3.2 Theoretical Reaction Models of 03 Production

The main reaction of 03 production is

$$01 + 02 \xrightarrow{K1} C\ (03) + D \qquad (1)$$
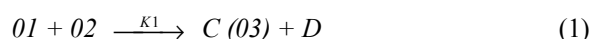
and the side reaction of 03 production is

$$01 + 02 \xrightarrow{K2} E \qquad (2)$$

where $C\ (03)$ denotes the main product, D and E the side products, $K1$ the reaction rate constant of the main reaction, and $K2$ the reaction rate constant of the side reaction. The reaction kinetics of 03 production is

$$K = Ae^{-E/RT} \qquad (3)$$

where T is the temperature (K); E is the activation energy; A is the frequency factor. E and A are the reaction kinetics parameters estimated either by experiments or calculated by a related empirical formula.

In fact, the reaction models of 03 production can be described by

$$K1 = K_{01}e^{-E1/RT} \qquad (4)$$
$$K2 = K_{02}e^{-E2/RT} \qquad (5)$$
$$R1 = K1*C_{01}C_{02} \qquad (6)$$
$$R2 = K2*C_{01}C_{02} \qquad (7)$$
$$dC_{01}/dt = -K1*C_{01}C_{02} - K2*C_{01}C_{02} \qquad (8)$$
$$dC_{02}/dt = dC_{01}/dt \qquad (9)$$
$$dC_c/dt = K1*C_{01}C_{02} \qquad (10)$$
$$dC_d/dt = K1*C_{01}C_{02} \qquad (11)$$
$$dC_e/dt = K2*C_{01}C_{02} \qquad (12)$$
$$dT/dt = 1/(Cp* \Sigma M)*(\Delta H1*R1 + \Delta H2*R2 + Q1 - Q2 - Q3) \qquad (13)$$

where $R1$- the main reaction rate, $R2$- the side reaction rate, T - the reaction temperature, R- the standard gas constant, $E1$-

the activation energy of the main reaction, $E2$- the activation energy of the side reaction, $K01$- the frequency factor of the main reaction, $K02$- the frequency factor of the side reaction, $C01$- the 01 concentration, $C02$- the 02 concentration, Cc- the concentration of the main product, Cd- the concentration of the side product D, Ce- the concentration of the side product E, Cp- the average heat capacity, ΣM- the total weight of chemicals inside the reactor, $\Delta H1$- the heat of the main reaction, $\Delta H2$- the heat of the side reaction, $Q1$- the heat of the reactor jacket, $Q2$- the cooling load of the reactor jacket, and $Q3$- the other cooling load.

3.3 Model of Assessing Operator's Performance

The evaluation model for analyzing operator's training results should be precise and objective. It should consider trainee's operation sequence, operation quality and safety at the same time [6].

The model of assessing operator's performance, based on his/her operation record on the new IPC-mode process simulator, is as follows:

$$S = WS \cdot SS + WQ \cdot SQ + WA \cdot SA \qquad (14)$$

$$SS = \sum_{i=1}^{n} SS_i \qquad (15)$$

$$SQ = \sum_{i=1}^{n} SQ_i \qquad (16)$$

$$SA = 100 - \sum_{i=1}^{n} SA_i \qquad (17)$$

where: S- the total score of trainee, SS- the score from correct operation steps; SQ- the score from correct operation quality; SA- the score from safety operation (no alarm); SS_i, SQ_i and SA_i-the trainee's i-th step score from correct operation sequence, quality and alarm; WS, WQ and WA- the weighting factors for evaluating operation sequence, quality and safety; and n- the total operation steps.

3.4 Dynamic Compensation Method

As the dynamics of the small-scale chemical process is very complicated, it's difficult to accurately build the process dynamic model using the theoretical analysis method. Moreover, the final goal of this simulation work is to build an operator-training simulator, and the requirements of modeling accuracy are not very strict. In the operator-training simulation, when a process input is entered, it requires that the variation direction and trend of process parameters be the same as the real process [10]. The difference between the simulated process parameters and the real process is limited within the error range set by the simulator's technical specification. An operator-training simulator also requires its operation sequences and steps are in agreement with the process operation regulations. So a simple and useful dynamic compensation method is used to build the dynamic models of

this small-scale fine chemical production process. The first-order and second-order compensation method is usually used to calculate the amplitude gain and time coefficient of the process according to the initial steady state value and final steady state value of the process parameters and their transient responses.

The commonly used dynamic compensation equations for process modeling are:

$$Model_{dynamic} = \frac{1}{T_1 S + 1} * Model_{static}$$

$$(First\text{-}Order\ Compensation) \qquad (18)$$

$$Model_{dynamic} = \frac{1}{T_1 S + 1} * \frac{1}{T_2 S + 1} * Model_{static}$$

$$(Second\text{-}Order\ Compensation) \qquad (19)$$

where T_1 and T_2 are the time coefficient determined by the dynamic properties of the simulated process. Using equations (18) and (19), the process static models can easily be transformed into dynamic models.

The most commonly used dynamic compensation method for process simulation is Euler compensation method [9,10]. It has three steps in a simulation computation cycle.

Step 1: calculate the compensated variable X using its algebraic equations of the process static model.

Step 2: carry out Euler numerical integration using the following equation.

$$X = X_0 + H (X - X_0) / T \qquad (20)$$

where X denotes the compensated variable, X_0 the previous value of the compensated variable, H the time step length for integration and T the time coefficient for compensation.

Step 3: let $X_0 = X$ and repeat the computation cycle.

In order to keep the stability and accuracy of the Euler integration algorithm, the time step length H should be small enough. Generally, the time coefficient T for compensation should be kept at 10-1000. Normally, when the time coefficient of process model is small, T should be small; when the time coefficient of process model is large, T should be large.

4 Dynamic Link Library Functions

VC++ is the most commonly used programming language for developing the operator-training simulation software [12] due to its powerful visual and object-oriented programming ability. In this paper, a dynamic link library (DLL) function, called UserFunc.dll, is designed to fulfil the model calculation, training evaluation, accident simulation, dynamic data exchange with CENTURY STAR and other simulation training tasks. Then a comprehensive simulation training software package is developed by integrating the SCADA configuration software CENTURY STAR and the DLL function program.

UserFunc.dll is created by compiling and linking the VC++

source code program UserFunc.cpp, the head file UserFunc.h and other related files. The flow sheet of the program UserFunc.cpp is shown in Figure 2. The main functions of UserFunc.cpp are initialization, downloading configuration data to the model, model calculation and uploading the model calculation results to the configuration software CENTURY STAR. The head file UserFunc.h is used to set up data structure, declare external functions and define data types.
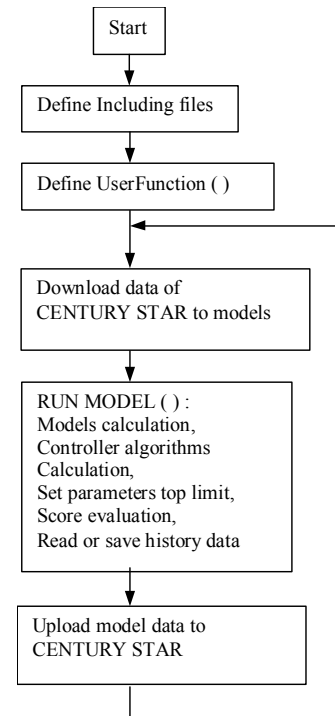
Figure 2: The flow sheet of UserFunc.dll program

5 Development of GUI and Command Language Programming

The SCADA configuration software CENTURY STAR is used to develop the graphical user interface (GUI) of the operator-training simulator. The GUI includes several diagrams of a simulated process flow sheets, a operation diagram of a manually actuated valve, a operation diagram of a PID controller and a tuning diagram of PID controller parameters, an alarm report diagram, a score evaluation diagram, a history trend chart and its type selection diagram, a time-scale setting diagram, a real time trend chart, an accident assignment diagram and etc. The programs corresponding to the displaying and operation of those diagrams are designed in the powerful command language of CENTURY STAR. A typical example of the simulated process flow sheet is shown in Figure 3.

In each simulated process flow sheet, a dozen of simulation training operation command buttons are set up, which are named as RUN, PAUSE, ACCIDENT, SCORE, TREND CHART, ALARM, SNAPSHOT, TIME-SCALE, STOP and process flow sheets display switching command buttons (including FLOWSHEET1, FLOWSHEET2, FLOWSHEET3
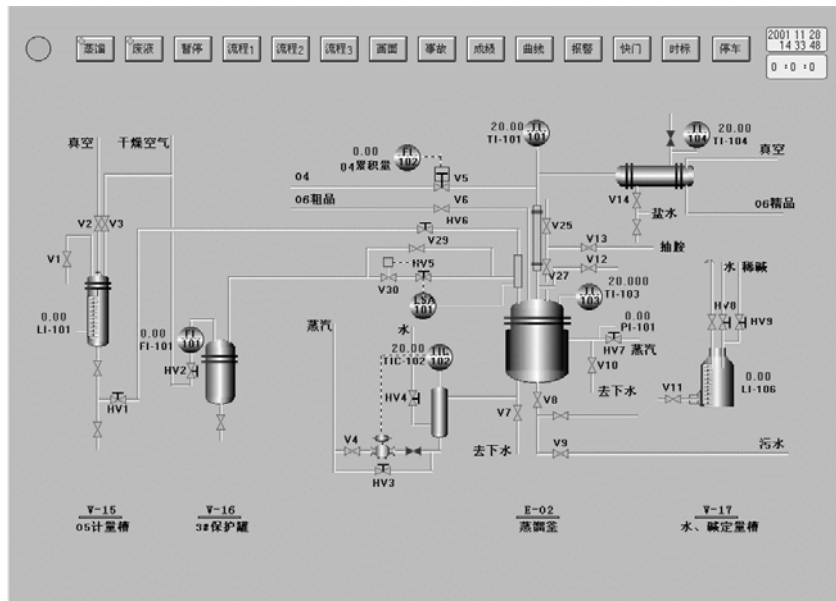
Figure 3: The simulated process flow sheet 1 of 06 distillation

AND FLOWSHEETS four buttons). The programs corresponding to the operation of those command buttons are also designed. They display the corresponding operation diagrams of command buttons, give operation commands and enter parameters. For example, when the CENTURY STAR starts to run, its application program is programmed as

```
Logon (  ) ;
Recipe Load ( "Initialization Recipe" ) ;
```

When the CENTURY STAR is running, its application program is changed to *UserDLL ();* In this way, the CENTURY STAR can initialize its running at first and then fetch the DLL function program UserFunc.dll running in parallel to accomplish the overall operation simulation functions of the small-scale fine chemical process.

The programs of the on/off valve V1 and the automatic controller TIC-102 in Figure 3 are designed as follows.

a. The program of the on/off valve V1

```
IF run command = = 1 THEN
    IF V1= = 0 THEN
        V1 =1;
    ELSE
        IF V1= = 1 THEN
            V1 =0;
        ENDIF;
    ENDIF;
ENDIF;
```

b. The program of the automatic controller TIC-102

```
IF (run command = =1 && tuner switch = =0) THEN
tuner switch=1;
tuner name="TIC-102"
tuner level No.=2;
unit = "°C"
set point SP= set point of TIC-102;
process variable PV= process variable of TIC-102;
manipulated variable MV = manipulated variable of TIC-102;
```

```
maximum value of tuner = maximum value of TIC-102;
selection of control method = control method of TIC-102;
ShowWindow("PID Controller Operation Diagram");
ENDIF;
```

By running the above programs, we can operate valves, controllers and switches in the simulated process flow sheets as operating the real process.

6 Operation Simulation Results

The small-scale chemical process operator-training simulator is validated and tested carefully by process technicians many times. After revision, modification and adjustment of the simulator's flow sheets, command language, process models and their calculation program, it is proved that this operator-training simulator can simulate the process flow sheets, the dynamic behavior of the process, the virtual operation of valves, switches and instruments very well. Furthermore, the simulation accuracy of the operator-training simulator can satisfy the process operator-training requirements at both the steady state and the transient state, and the simulator's operation sequences, steps and actions are in accordance with the real process operation regulations.

For example, some operation simulation results of the raw 06 distillation to produce fine 06 are shown in Figure 4. In Figure 4, the real-time trend charts of the top temperature (TI-101, red), kettle temperature (TI-103, blue) of the 06 distillation, and the temperature of the steam-water mixer (TIC-102, green) are illustrated for the whole 06 distillation period. The process operation experts confirmed that the temperature curves shown in Figure 4 were very close to the real distillation temperature curves. These curves can vividly simulate the operation results of the 4 distillation periods: heating to start distillation, output of the overhead distillate, shifting of different kind distillates and halting distillation.

After many careful examinations by the process technicians, this simulator has been used to the operation training of dozens of process operators before they start to operate real processes. The simulator operation-training practice helps them to further understand the processes and their flow sheets, get familiar with the process operation regulation, and remember how to prevent from and deal with production process accidents in a very short training course. In brief, the simulator has achieved very good training results in training practice.
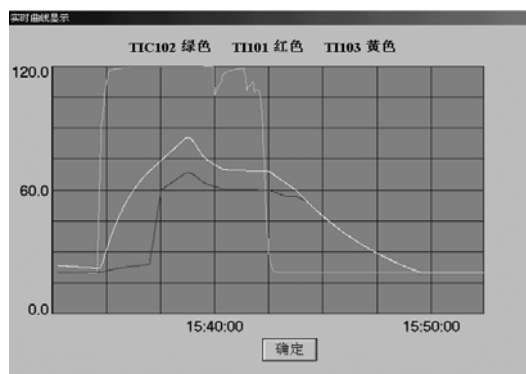

Figure 4: Temperature curves of the simulated 06 distillation

7 Conclusions

Based on the careful study of the characteristics of small-scale fine chemical production processes and their computer simulation training requirements, the main structure, the mathematical model, the graphical user interface and implementation technology of an IPC-mode simulator for chemical production process operator-training have been thoroughly discussed in this paper. A novel type IPC-mode operator training simulator for small-scale fine chemical production processes has successfully been developed, which can be used to train process operators, support process operations and implement process optimization. The training results show that the simulator satisfies the process operator-training requirements very well. This implies that the design method of the new IPC mode simulator developed by this paper is effective and feasible, and it also possesses good theoretical and technological significance for the development of other process operator-training simulators.

Acknowledgements

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