An Application of Dynamic Simulation in Advanced Control

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Abstract

There are three primary systems in which process simulators apply: online, quasi-online, and off-line systems. In regard to conventional process simulators, both steady-state and dynamic simulators have been used in off-line systems.

This article, however, mainly discusses the dynamic simulators applied in the online system with the following example of a "polypropylene" polymerization process. First-principle-based rigorous models were constructed in a dynamic simulator with unique functions, which accelerate the calculations of each unit model, physical properties, and especially the pressure flow network balance of the entire plant. The actual operation data was then incorporated into the on-line system, and based on the data, an initial condition was created for the models. Simulation was performed based upon the initial condition employing a number of potential recipes. After having found the optimum recipe, it was applied in actual operations. An integrated system was meticulously constructed, and as a result, the plant operations made significant improvements; thus greater laborsaving efficiency and productivity were achieved.

This demonstration was successfully proven in actual operations by Mitsui Chemicals Inc., a major Japanese chemical company.

1. Introduction

In recent years, tremendous changes have occurred in the application method and functions of dynamic simulators. The application of dynamic simulators has extended to the areas of design/analysis, operation training, operational support and optimization. Demand for functions, which include 1) the modeling of more rigorous plants based on first principles of chemical engineering, 2) the modeling of control systems that perform identically to actual ones, and 3) a connection to DCSs and real-time systems such as process computers, have drastically increased. In such circumstances, because of the significant improvements in computer calculation ability and graphic user interfaces, coupled with the need of safer and optimal plant operations, it is becoming relatively easier to develop rigorous dynamic simulators.

In this article, we will introduce the dynamic online system which achieved automation and optimization of product grade transitions in the polymerization process. First will be a description of the application areas of dynamic simulators followed by their functions.

2. Application Areas of Dynamic Simulation

Dynamic simulation technology will play a very important role in achieving safer and optimal plant operations. As shown in Figure 1, dynamic simulators are applied in three principal systems: off-line, quasi-online, and online systems.

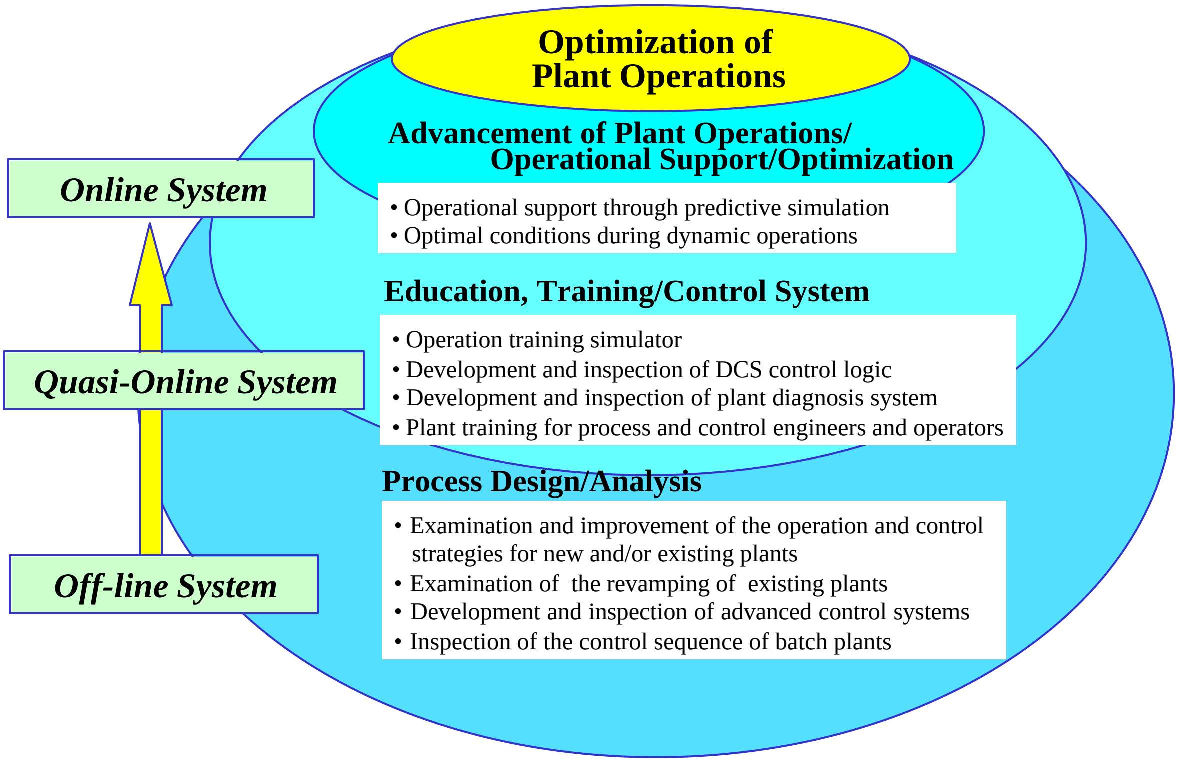

Figure 1. Application Areas of Dynamic Simulation

(1) Off-line Systems for Process Design and Analysis

In off-line systems, results obtained from the dynamic simulator in the system are not immediately applied to actual plant operations. This conventional method is used to 1) examine and improve the operation and control strategies for new and/or existing plants, 2) examine the revamping of existing plants, 3) develop and inspect advanced control systems, and 4) evaluate the control sequence of batch plants.

(2) Quasi-Online Systems for the Education/Training and Development of Control Systems

In the quasi-online systems, the results obtained from the dynamic simulator are applied to simulated plants. Usage of this system include 1) developing and inspecting DCS control logic and plant diagnosis systems, and 2) training process/control engineers and operators.

(3) Online Systems for the Advancement of Plant Operations, Operational Support and Optimization

The results obtained from the dynamic simulator in the online system are fed back to the actual plant in real-time. This online system is used to 1) support operations based on predictive simulation and 2) optimize conditions during dynamic operations that occur at continuous process plants. The modeling of an entire plant and control systems, the integration of a plant model with real-time machines and the estimation of parameters and initial condition values corresponding to the actual plant data are three crucial factors in this application.

A plant model constructed in the dynamic simulator is regarded as a base in all three areas. And because of the enormous amount of financial and intellectual investment made in the development of the plant model, it is important that the infrastructure, which enables the model to be commonly used, be provided in the simulation process.

3. Functions Required for Dynamic Simulators

This section outlines functions of the dynamic simulator (Visual Modeler®), which was developed for common utilization in off-line, quasi-online, and online systems.

(1) Model Fidelity

The unit models constructed in dynamic simulators (e.g., distillation column, heat exchanger, etc.) require the same or higher level of accuracy than those in steady-state simulators. For example, the vapor-liquid equilibrium and heat balance calculations are performed at each tray in the distillation column, and the internal pressure caused by changes in the vapor hold-ups is calculated. For the heat exchanger, the dynamic simulator must have the ability to describe the inner conditions in detail because of its dynamic characteristics. The key factor in plant modeling is pressure. To duplicate pressure changes in the model (as nearly as possible), the simultaneous equations representing a relation between the pressure and flow rate of the entire plant must be solved, and this balance calculation must be performed at all times. Thus, it is essential that the dynamic simulator function with the ability to automatically extract the relation of the pressure and flow rate and solve it at high speeds.

(2) **Scale of Simulation**

To examine training and operation strategies, dynamic simulators require modeling of control equipment, pipe lines, hand-valves, and safety and auxiliary equipment for the operations in dynamic circumstances such as shutdown and startup. Thus, for the same type of plant, dynamic simulators require 10 to 100 times more units than steady-state simulators. Some large-scale plant simulators consist of several thousand units. To handle such large-scale plants, more efficient model developing environments and the modeling technology that enables high-speed executions are required.

(3) **Standard and User Unit Models**

Units required in dynamic simulators but not in steady-state simulators include tanks, safety valves, check valves, time lag pipes, measuring instruments and control equipment. While the same results can be obtained from one unit model in steady-state simulators, dynamic simulators often require each model to function identically to actual conditions because of its dynamic characteristics and different handling procedures in operations. For that reason, more than 200 different types of unit models (processes and instrumentation) are registered in the standard library of the dynamic simulator. Although various types of standard unit models to meet different conditions are typically included, the cases where these models are insufficient occur more frequently in the dynamic simulator. The reasons are, for example, 1) for the reactor and special separator, the reaction mechanism and structural features are easily reflected as discrepancies in models; and 2) in addition to the loop controller, special types of models such as sequence control and/or the models with a calculation function of all kind are required. It is, therefore, of utmost importance that there be features which allow users to add unit models to the library according to their needs. The dynamic simulator features functions to satisfy this purpose, and features an effective function for model description (EQUATRAN®, equation solver language). A major advantage of this function is that the user is never required to do any programming.

(4) Execution Functions

Simulation enables execution in real time and interactive responses per second. These features are extremely important especially when training simulators are used as real-time systems. They also become very effective in situations where engineers use them for analytical purposes and want to feel a sense of realism.

This dynamic simulator uses a high-performance computer to calculate a large-scale simulation with rigorous models on a per-second basis, featuring unique functions to accelerate the calculations of each unit model, physical properties, and the pressure flow network balance of the entire plant.

(5) Engineering Environment

When dealing with a large-scale plant, the development job becomes much easier if it is divided into groups. One plant can be divided into several process models, allowing engineers assigned in each section to perform development tests independently. After all the tests are completed, they are combined into an integrated plant model.

To make the development work more efficient, process flow diagrams (PFDs) are used for the construction and execution of a plant model. Process models are created by 1) selecting necessary unit models from the library menu, 2) placing them on the PFD, 3) connecting them with streams and signal cables, and 4) inputting respective parameters (size and characteristic data) for each unit model. Figure 2 shows an example of the model execution panel. It uses the same PFD as that in the model editing panel; thus, the entire handling of execution, including running and pausing operations and changing parameters for each unit models can be performed at any time on this panel.

(6) DCS Connection

The DCS connection is indispensable to realize a high-performance training simulator from which a sense of realism is obtained; this makes it possible to directly develop and inspect the control system in the DCS.

(7) Graphic Environment for General Users

As an application system environment where simulators can be used for many different purposes, the graphic panel that allows users to design graphics at their discretion and the interface that enables simulation data to communicate with other applications must be provided. As other application systems, simple-type training simulators and the simulators for process education, operational support and optimization are included.

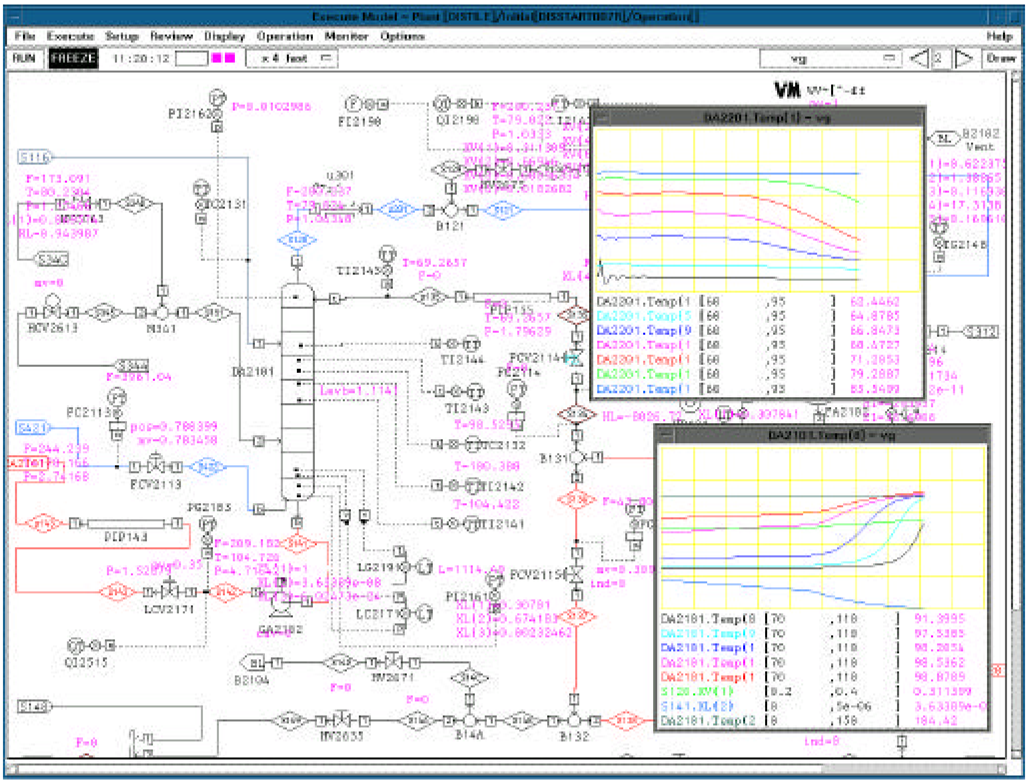

Figure 2. Model Execution Panel

4. Actual Example of the Optimization of Grade Transitions for Polymerization Processes in the Online System

In the polypropylene process where product grade transitions are frequently performed, the major objectives that must be achieved are reducing the transition time with proper production schedule, stabilizing reactor behavior for safe operations and minimizing off-spec production. This section describes the role that the dynamic simulator actually played in the construction of a system and that contributed to the automation and optimization of grade change operations.

4.1 Process Overview and Grade Change Operations

Figure 3 illustrates the continuous liquid pool processes of polypropylene. In this example, a monomer, comonomers, hydrogen and a catalyst are continuously fed to a continuous stirred tank reactor (CSTR), and the polymerization is conducted in the liquefied monomer in the CSTR. To maintain constant reactor temperatures, the heat of polymerization is removed using a cooling jacket of the reactor and/or the condenser. The catalyst implemented here is a high activity Ziegler-Natta catalyst. The melt index (MI) and the amount of comonomers, such as ethylene, contained in the polymer are controlled by adjusting the concentration of hydrogen and comonomers. The catalyst activity is also affected by the concentration of the two materials; thus when changes in the molecular weight and/or the amount of comonomer during a grade transition, the catalyst rate must be adjusted accordingly in order to remain the reaction rate constant. The grade change operations require a lot of time and efforts because the amount of each material injected to the reactor must be adjusted to maintain inner conditions of the reactor within a range where removal of the heat can be controlled.

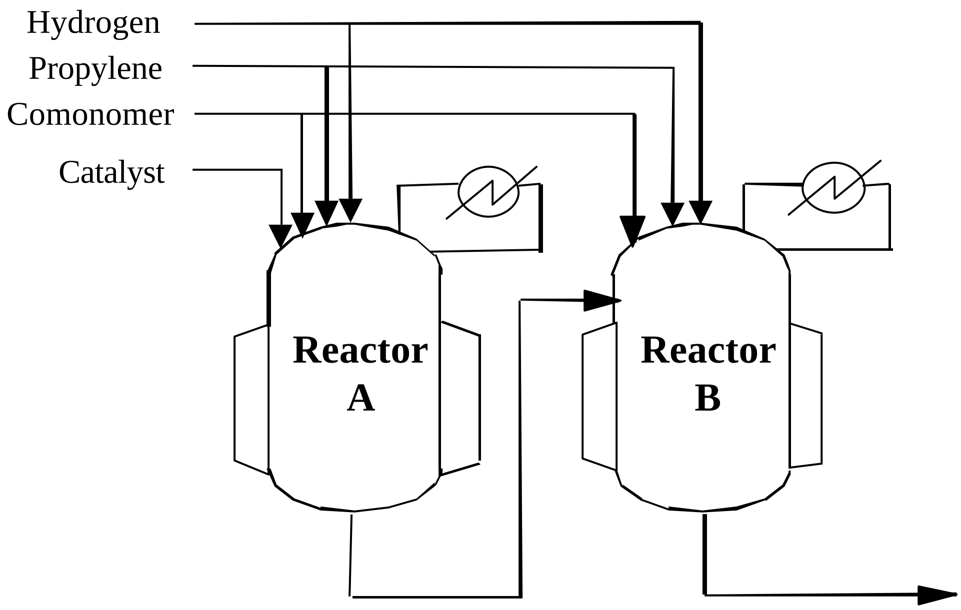

Figure 3. Continuous Liquid-Pool Process Flow

4.2 System Configuration Required for Grade Transitions

As shown in Figure 4, the grade transition system configuration consists of two components. The first component represents a DCS and a process computer for the automation of grade transitions, and in the second, a simulation computer is utilized to achieve optimization of grade transition patterns.

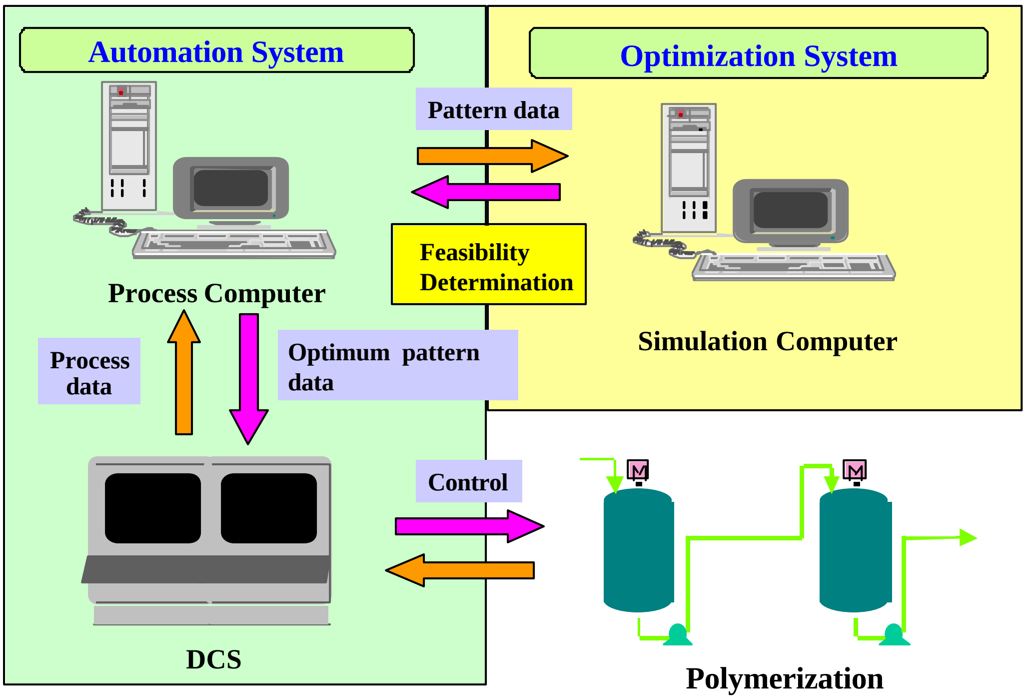

Figure 4. System Structure for Automatic Grade Transitions

(1) System for the Automation of Grade Change Operations

The process control is performed in the DCS, and prior to the DCS is a process computer, which is used to achieve advanced control (e.g., grade transitions) and operating support functions (e.g., detection of abnormal conditions). The process computer contains the following databases for grade transitions.

- The modification logic required to create transition pattern data of setpoint variables
- The default setpoint variables for the catalyst rate, the amount of monomer, comonomers, hydrogen, etc. for each grade

The following operating procedures are performed during a grade transition.

1) With the modification logic, automatically creating transition pattern data from the current setpoint variables and the default setpoint variables of the post-grade transition.
2) Sending a command from the DCS console to start a transition.
3) Transmitting transition pattern data from the process computer to the DCS.
4) The grade change operations are automatically performed at the DCS based upon the transition pattern data. In addition to the loop control, the sequence control is incorporated in the DCS for grade transitions (modifications of setpoint variables) to be safely performed. In any situations where the continuation of an operation is likely to interfere with the safety of the plant, it is imperative that the operation be immediately stopped and the situation be notified to the operator.

(2) System for the Optimization of Grade Transition Patterns

The key factor for the optimization of a grade change is to reduce the amount of off-spec product produced during a grade transition. To achieve this, it is sometimes required to temporarily increase the feed rate of comonomers and hydrogen and then reduce the rate to the fixed level once their concentration levels have reached normal. However, this action could cause significant changes in the catalyst activity resulting in situations where temperatures cannot be controlled. Thus, it is important that the constant rate reaction and the optimum condition of the reactor are maintained while a grade transition is being performed. In the dynamic simulation system, which was developed to achieve the goal of creating effective and optimal grade transition strategies, normal conditions are registered for each grade as default, and either the registered normal conditions (referred to #1 below) or the normal conditions modified in response to the actual operating conditions (referred to #2 and #3 below) is used as an initial condition. The execution of the dynamic simulation is effectively performed based upon the initial condition and the transition pattern data created in the process computer.

The following are three possible simulations.

1) Standard Simulation

This is a case study mode executed for the registration and modification of grade transition pattern data. After the transition patterns between grades are determined by comparing the typical operating conditions (e.g., cooling water temperatures and the catalyst activity) with the standard operating conditions of the pre-and post-grades, they are registered into the process computer.

2) Simulation to Verify Before a Transition

This mode is used to verify the actual transition pattern after the operating condition data immediately prior to the start of a grade transition is downloaded from the process computer. Of all the patterns registered in the mode (1), the optimal pattern, which is applicable in the actual plant and offers minimum transition time, is selected and determined.

3) Simulation for Actual Comparison

This mode is used to fine-tune and inspect models, and compare simulation results with actual operation data (e.g., SV value) stored in the process computer.

The following is the operations performed during a grade transition, and the block flow diagram describing the actual grade transition system is shown below.

1) Receive operating condition data immediately prior to the start of a grade transition.
2) Execute the simulation that provides normal condition values in response to the operating condition data (calculation of initial values).
3) Receive transition pattern data from the process computer.
4) Perform a simulation based upon the initial values and transition data, and evaluate the data to see if it is executable in the actual plant.
5) Repeat the above two steps 3 and 4 until the optimal transition pattern is found.

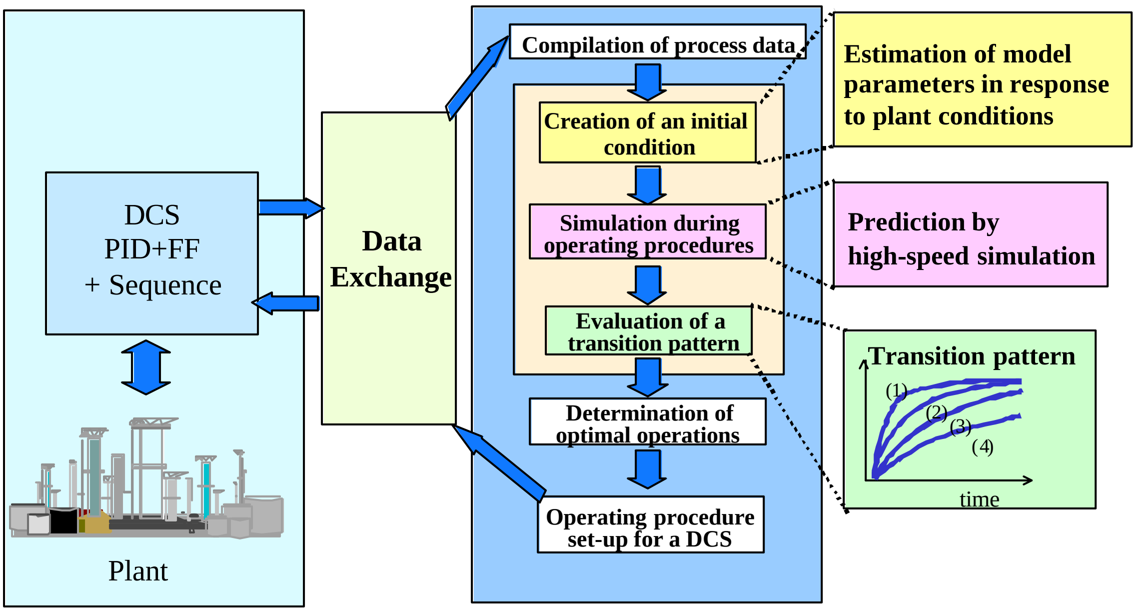

Figure 5. Determination of Optimal Operating Procedures
and Integration with Control Systems

4.3 Simulator Overview

This section describes the dynamic simulator contributing as a key factor in the constructed system. The components of the dynamic simulator include: plant models and control system models.

(1) Plant Models

The plant models represented in the dynamic simulator include polymerization reactors, heat exchangers, control valves and measurement equipment. In the reactor model, the reaction rate is calculated through equations considering the occurrence of changes in the concentration of the catalyst, monomer, comonomer, hydrogen and etc. In addition, the average molecular weight that expresses the physical properties of a polymer and the copolymer compounds are calculated in the dynamic simulator. The controlling of the reactor temperatures is the key factor in the polymerization processes. Thus, the heat transfer coefficients of the heat exchanger and the characteristics of the control valves are carefully fine-tuned so that the temperatures are controlled in the same manner as in the actual processes.

(2) Control System Models
The modeling of DCS logic control, which functions in the same manner as the actual one, is performed in the dynamic simulator. The actual control parameters are also utilized.

(3) Simulator Fidelity
The dynamic simulator must have the ability to determine if the resulting set of transition pattern data is applicable to the actual plant. Fidelity and reliability are the two most important factors required in the dynamic simulator. For this reason, thorough testing and inspection of the models were conducted in our application to ensure that their qualities were satisfactory. Figure 6 shows the results of the heat of reaction in two different reactors A and B during a grade transition, comparing the actual data and simulation calculation values. It is clear that the actual and simulation data are very closely matched in both reactors.

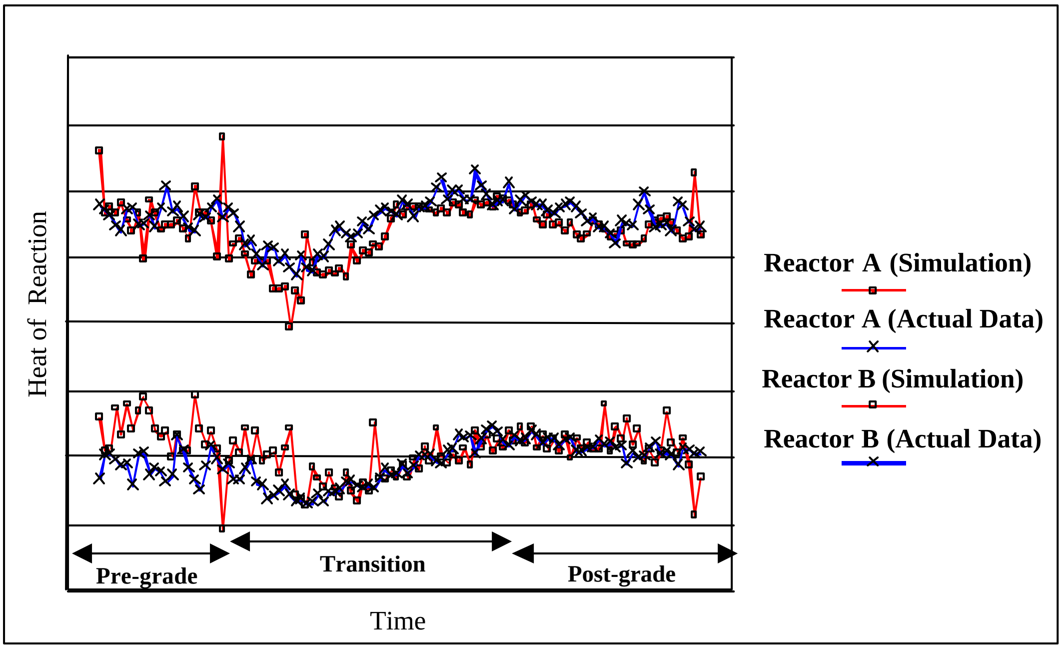

Figure 6. Heat of Reaction during a Grade Transition

4.4 Achievements

The following are the effects of this system for the automation and optimization of grade transitions.

1) After the optimization of a transition pattern was implemented through simulation, plant operations were stabilized and the transition time was minimized. Thus, the production of off-spec products was effectively reduced, resulting in a significant reduction of the total production cost of the products.

2) Through the automation of grade change operations, the operators' tasks were reduced and standardized.
3) It became easier to create new grade transition patterns.
4) Delivery of the technology information on the creation of transition patterns was successfully achieved.

5. Conclusion

It is of utmost importance that the plant model constructed in a dynamic simulator be commonly applied in the off-line, quasi-online and online systems as a "simulated plant." We particularly believe that it is an extremely effective approach to fully utilize the dynamic simulator for operational support and the development of advanced control to realize the advancement of plant operations.