Advances in Chemical Process Control and Operation

– A view experienced in joint university-industry projects–

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Abstract

A state of the arts in Japanese chemical process control is reviewed based on experience in applying advanced process control schemes to several industrial chemical processes. The applications validate model predictive control (MPC), the most popular advanced control scheme in the process control community, as, indeed, a powerful and practical control algorithm. However, at the same time, it is elucidated that MPC can solve only the control algorithm part of the problem and one needs chemical and systems engineering aspects to solve the entire problem. By illustrating several industrial process control problems, the need for chemical engineering aspects as well as the future direction for process control are addressed, especially in light of current attitudes toward product quality.

Keywords: Process control; predictive control; quality control; on-line inferential system; plantwide control

1. Introduction

The last several years have heard many discussions on what the present problems are that Japanese industries face and how high-level production systems in the next generation should be for the 21st century. Three major problems addressed currently are[1]:

1) the aging of society and shortage of young workers,
2) diversified requirements for products,
3) intensification of international competition.

The strategies taken by the industry to cope with these problems can be expressed by four factors:

a) production information integration,
b) hyper-automation,
c) Just-In-Time production (timely production) and reduction of inventory cost,
d) human resource recruitment.

To execute these strategies, the application of advanced process control and development of computer integrated manufacturing systems as well as strategic information systems have been steadily progressing in the process industries. In this movement, process control is regarded to be one of the key technologies in the next-generation production systems and is being further advanced so as to realize flexible production systems with high quality products.

It should be noted here that model predictive control (MPC) became known in the late 1970s to early 1980s. It has accomplished industrial success in many chemical process control applications and has achieved a significant level of acceptability in process control with contributions of improvement of operating efficiency and profitability[2].

MPC is indeed a powerful method but it solves only the control algorithm part of industrial problems with chemical and systems engineering aspects absent in the algorithm. One needs these engineering aspects besides an advanced control algorithm in order to develop a practical process control system.

Stephanopoulos[3] notes that process control systems design is carried out in five major steps:

1) define operational objectives,
2) identify the measured variables,
3) identify the possible manipulations,
4) determine the control configuration and strategy,
5) design the controller.

In other words, the development of a practical process control system is not complete with only the PID controller design and installation of an advanced control algorithm. To complete it, the integration of the control technique with process design, monitoring, and diagnosis techniques, based on process understanding, is necessary.

In this paper, the current and future needs of process control are addressed by illustrating several practical examples experienced in joint university-industry studies. We have had exceptionally good collaboration with the corporate sector and have relied on such collaborations in addressing the current and future direction of process control. These examples given are mainly from polymerization reactor plants and our attention is especially focused on the product quality.

2 Quality modeling & On-line quality inferential system

2.1 Quality Modeling

The changes in customer expectation for product quality have directed the industry's attention to the importance of product consistency. The demand for product consistency is going to become greater and the manufacture of consistent high-quality products using minimum resources and creating little waste are key elements of the competitive edge for industries.

In order that process control engineers commit themselves to product quality improvement, the study of quality modeling should be advanced. Quality is not always given by physical and chemical properties, but is sometimes given by empirical expressions. For such cases, the quality model is indispensable for translating information on product quality requirements into specifications for physical state variables in the process. The modeling of the quality and a method of integrating the quality model with a conventional process model are crucial to attain a good quality control system.

2.2 *On-line quality inferential system*

In polyethylene polymerization processes, the polymer product quality is often quoted in terms of rheological properties, e.g., the melt index (MI), viscosity and so on. Due to the lack of an on-line sensor for the polymer quality, it is occasionally evaluated off-line in quality laboratories, usually taking two or three hours to obtain an evaluation result. These infrequent measurements with large time-lags hinder the appropriate countermeasures to disturbances in the polymer quality and often result in a wide variation of product consistency.

One of the recent activities to overcome the difficulty mentioned above is to develop quality models and then construct an on-line inferential system that can predict the quality in real time from off-line measured polymer properties and on-line measured state variables. In the system, a quality model that can infer the polymer quality (MI) from state variables of the reactor, i.e., monomer and hydrogen concentrations, is developed and utilized in a filtering scheme, such as a Kalman filter and recursive estimation scheme.

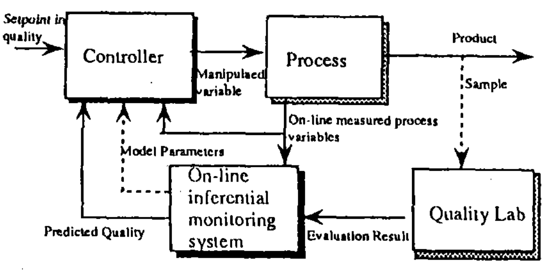


Fig. 1 On-line inferential quality control system

When a new measurement of polymer quality becomes available from the lab, model adaptation is performed based on the difference between the measurement and the predicted value given by the quality model. After each update, prediction of the quality is made by successive evaluation of quality model with on-line measured process variables until the next measurement of quality is available from the lab. The predicted value is used on-line to determine the control actions, as illustrated in Fig. 1.

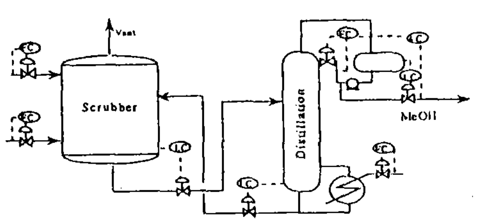
McAuley and MacGregor developed an inferential system for the Linear Low Density Polyethylene (LLDPE) process by using a theoretically-derived quality model[4]. On the basis of an empirically derived model, Watanabe et al. developed an inferential system for the High Density Polyethylene (HDPE) process[5]. Koulouris et al. illustrated the ability of Wave-Nets, which is an artificial neural network with basis functions drawn from the family of wavelets, to capture the functional relationship between the polymer quality (MI) and process variable. They proved its potential as an on-line inferential scheme to predict the quality in real time for polyolefine polymerization processes[6].

In three cases, the quality models are different each other but the basic structure of the inferential systems is common to all three. The structure illustrated in Fig.1 is applicable to other chemical processes where the quality cannot be measured often, but needs to be controlled on-line. Ohshima employed the structure to develop an inferential system for pyrolysis plants to monitor the tube-wall temperature on-line[7]. The structure offers one of the most promising frameworks for an integrated information system that utilizes lab data for efficient plant operation.

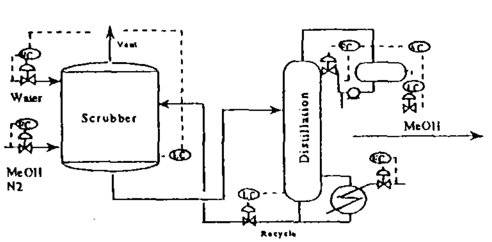
3. Plantwide control and optimization

3.1 *Plant wide control*

Downs introduced a simple example to illustrate the necessity of plantwide control[8]. His example plant consists of a scrubber and a distillation column, as illustrated in Fig. 2. In this plant, a 900 mol/h nitrogen offgas containing 10 % methanol is scrubbed by feeding 10 mol/h fresh water to the scrubber and then the water containing the methanol is fed to the distillation while the scrubbed nitrogen is vented. The distillation column has to be controlled to concentrate the methanol to a 90 % methanol and 10 % water distillate product. The bottom product of the column is returned to the scrubber. For this plant, he shows two candidates of control system, which are illustrated Fig. 2-a and 2-b, respectively.



2- a Control strategy A



2-b Control strategy B

Fig 2 Methanol recovery plant and control strategy

The difference between the two systems is found only in the control loop for the scrubber. In the control system drawn in Fig. 2-a, level control of the scrubber is performed by manipulating the feed to the distillation column. Conversely, the other system does it by manipulating the feed flow rate of fresh water. The control system drawn in Fig. 2-a cannot control the whole plant against a disturbance in feed flow rate and/or composition of nitrogen off-gas. If the ratio of feed flowrate of methanol and water is changed from the 9/1 ratio, which is the ratio of methanol to water leaving the plant, the water is either accumulating or exhausted at the scrubber, because the component inventory of water is not self-regulating for the system in Fig. 2-a. That is, the control strategy illustrated Fig. 2-a will not work from a plantwide view point, even though the control of the individual unit might be satisfied.

This is a simple example but clearly illustrates that the total process is not merely the sum of units and the necessity of selection of control strategy from plantwide control.

3.2 Plant wide optimization

To deal with diversified products and customer requirements, not only batch but also continuous chemical processes are obliged to produce different grades of product by changing operation conditions.

For example, a large-scale pilot plant of impact polypropylene polymerization illustrated in Fig. 3 has to produce more than twenty different grades of polymer in the same reactor train. However, such grade changeover creates the potential for producing large amounts of off-specification polymer. Therefore, it is crucial to change the operating conditions as safely and quickly as possible. For this purpose, an optimal transition path has to be found within the feasible operating region, which is usually tightly constrained by the hardware capability, and product properties' requirements.

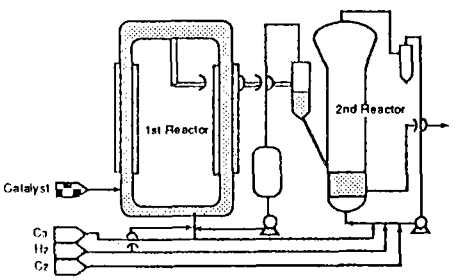
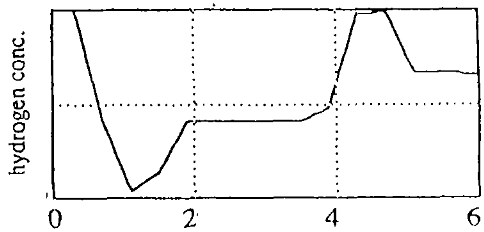
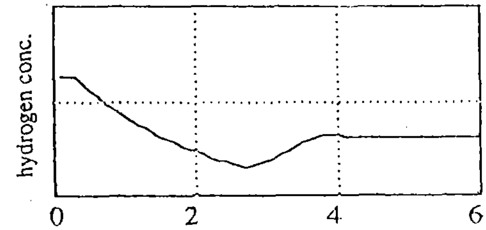


Fig. 3 An impact polymerization plants

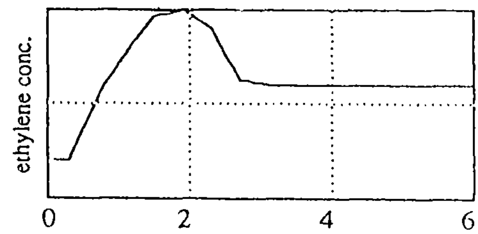
An optimal trajectory for the two reactors in the impact polymerization plant is illustrated in Fig. 4-a, b, and c[9]. As can be seen in these figures, the optimal grade changeover is not achieved by simply changing the operating conditions from the steady state value of one grade to another.



4-a Optimal hydrogen conc. change of the 1st reactor



4-b Optimal hydrogen conc. change of the 2 nd reactor



4-c Optimal ethylene conc. change of the2nd reactor

Fig. 4 An optimal changeover trajectory

The optimal policy for individual unit operations does not necessarily render the optimal policy for the whole process. Though the example of a particular polymerization is discussed above, a similar situation occurs at other chemical plants.

In the future, a plant wide optimization and control are much more strongly required as process integration advances.

4. Coordinated control

Usually, the number of the input variables available to be used in a control system is larger than the number of output variables to be controlled. There many chemical processes where controlling output variables by multiple manipulated variables is required to improve dynamic control performance while satisfying input constraints.

Again, the polymerization reactor is a typical example. At a polyethylene polymerization reactor, the ethylene concentration in the reactor needs to be controlled in order to maintain the polymer quality at a desired level as mentioned at the previous section. The feed flow rate of catalyst can be used to control the ethylene concentration in the reactor. However, it is dynamically slow because of constraints and has a large uncertainty in both the feed flow rate and the dynamics. The ethylene feed flowrate is an alternative that is dynamically preferable (fast) compared with that of catalyst feed flowrate. However, from the steady state point of view, the ethylene feed flowrate is equivalent to the production rate of the polymer. Therefore, it should be kept near a designated value. As such, it is desired to control the ethylene concentration while keeping the ethylene feed flowrate near a desired value by using both input variables simultaneously and in a coordinated way, as illustrated in Fig. 5. That is, the process needs a control system that can turn off the ethylene feed flowrate control and bring the flowrate back to the designated values as the effect of the catalyst feed is felt on the ethylene concentration. A classical example of such a control scheme is override control. Recently, more sophisticated control schemes achieving this objective have been developed, such as Valve Position Control [10] and Coordinated Control [11].

As we can see in this example, it becomes necessary in future process control to design a multivariable control system by prioritizing manipulated variables and control loops according to constraints as well as dynamics of the inputs.

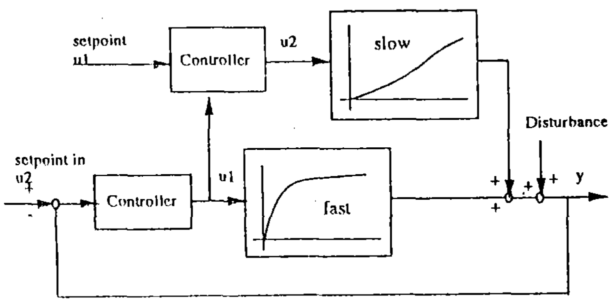


Fig. 5 Coordinated Control Structure

5 Control and modeling for multirate sampled systems

In many chemical processes, not all output measurements are available at the same sampling rate and not all input variables are available to be manipulated at a uniform rate of action. As described in the previous section, the polymer quality is measured off-line occasionally at a quality lab. The sampling rate of the quality is less frequent than the conventional P.T.L.F. measurements i.e., Pressure, Temperature, Level, and Flow measurements, and they may not be equally spaced in time. Furthermore, the direct feedback control of concentrations becomes necessary to keep the polymer quality at a specified level. The concentrations are usually measured by gas chromatographs and these measurements require a slower sampling rate than P.T.L.F. measurements. If all the control actions are synchronously performed at the slowest sampling rate, the control system cannot quickly attenuate disturbances in other, more frequently sampled outputs, such as temperature and pressure.

Normally, a multi-loop control strategy is employed to control processes where outputs are measured at different sampling rates. However, a multi-loop control strategy cannot provide the best control performance for those processes having strong interactions between inputs and outputs. Therefore, multirate multivariable control is required.

The study of multirate control systems began in the early 1950s for the aircraft control. There has been a great deal of research on stability analysis that employs either a transfer function or state-space description. But, few applications have been seen in process control. Recently, Gopinath and Bequette proposed a design method for multirate model predictive control of a SISO system where the output measurement is performed less frequently than the corresponding input action [10]. Ohshima et al. also proposed a multirate multivariable control algorithm as an extension of Model Algorithmic Control and applied it to the impact polymerization reactor [11].

Control techniques for multirate sampled processes have steadily progressed, however, the modeling techniques for these processes are not cultivated. Even though time series models, such as ARX, ARMAX and CARIMA models, are popular and practical linear representations of the process, few modeling schemes that can develop these models from multirate sampled time series data are established. As the demand for quality improvement grows higher and the necessity of multirate multivariable control systems becomes larger, the establishment of modeling techniques for multirate sampled data is much more indispensable.

6. Application of model predictive control and its limits.

Model predictive control has emerged and been acknowledged as a powerful and practical control algorithm. We have applied model predictive control to several industrial problems, listed in Table 1, which are relevant to the topics that we mentioned above.

Table 1. Industrial application of MPC

Process	Object	Approach	Issues	future problems
Optical Fiber Spinning Process	Diameter Control	˙Step Response model ˙FF/FB Control	Multiple Inputs system	Redesign at the different Spinning Speed
Fatty Acid Distil. Train	Composition Control	˙Step Response model ˙M P C with Adaptive function	Feed Disturbance Rejection	
GaAs single Crystal (LEC)	Crystal Diameter Control	˙Step Response model ˙M P C	Inference of Diameter.	not available for Small Diameter Crystal
Rotary Dryer	Quality Control	˙Step Response model ˙2x2 MPC	How to deal with D.P.S	not available at low production rate
Polymerization Reactor (polybutene)	Composition Control		Modeling from normal operation data	not complete
Polymerization Reactor (Impact copoly.)	Quality Control	˙Step Response model ˙3x3 Multirate MPC	Multirate sampled system Optimal Grade Changeover	no universal model for all grade
Polymerization Reactor (Polyethylene)	Quality Control	˙FF/FB IMC	Inference of quality Multiple Inputs	no universal model for all grade

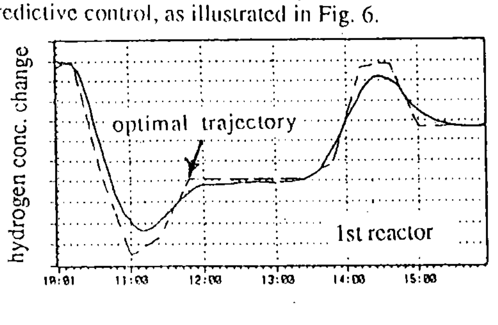
MPC could solve the control algorithm part of process control problems. However, there remain several problems that have to be solved from the chemical engineering aspect. This section addresses which part of the control problem could be solved by MPC and which parts could not.

In the optical fiber spinning process, by carrying out an open-loop step response test, the dynamics of the process were identified and feed forward and feedback control was constructed to keep the fiber diameter at a specified value. A model-based approach was taken for realizing the control structure. The difficulty we confronted during the development was the choice of the manipulated variables. The selection of the inputs to use in feedforward and feedback relied on the judgment and experience of the company's engineers. No general guideline to determine the control strategy could be derived. In addition, the system had to be redesigned when the spinning speed of fiber was increased.

The diameter control of the Gallium Arsenate single Crystal process was also carried out using model predictive control. However, a major difficulty was the lack of an on-line sensor of diameter. As such, an inferential control system was needed.

Similar difficulties appeared in a rotary dryer control problem[14]. In order to maintain the quality of a special material at the desired level, the temperature profile in the dryer had to be controlled. Instead of dealing with the partial differential equation model and a distributed parameter control system, the process could be treated as a lumped parameter system by controlling the critical drying point. The critical drying point is an inflection point of the temperature profile where the drying mechanism changes from a constant rate of drying to a decreasing rate of drying, although it is unmeasureable. By developing an inferential control system for the critical point, conventional model predictive control could be applied.

For polymerization reactor control, four different reactors were studied. The impact copolymerization process, which is illustrated in Fig. 3, is one of the multirate output processes, where the pressure and the monomer concentrations in the reactor are to be controlled. However, the sampling rate of the concentrations is less frequent than the pressure and temperature measurements. A multirate model predictive control scheme was developed by modifying conventional MPC and applied it to the polymer process. For this process, dynamic optimization was also considered in order to determine the optimal grade changeover. The optimal trajectory of the grade changeover operation, which was calculated by solving SQP on a workstation, is illustrated in Fig. 4. The tracking control was performed by conventional model predictive control, as illustrated in Fig. 6.



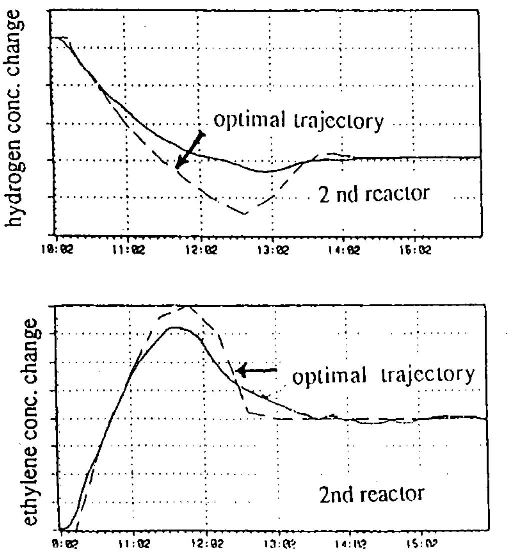


Fig. 6 Realization of optimal trajectory by MPC

The result shows the superior performance of MPC. However, a real-time optimization is required in the future since the calculated trajectory was no longer optimal once the state of the reactor differs from the trajectory. The receding horizon type optimization is promising when the process has a reasonably large time scale for dynamic behavior so that a solution of the optimization can be calculated for each controller execution.

For the polybutene reactor, a multirate sampled control system was needed as well as the on-line optimization. However, the development of the control system was retarded because of difficulties in developing a suitable model from the closed-loop controlled process data, i.e., normal operational data.

There are further difficulties which might be solved by the integration of the knowledge-based approach with model-based approach.

For example, in the case where MPC was applied to the impact copolymerization reactor, a step response model was prepared for each grade. For a reactor, more than twenty to thirty linear models were prepared to cover the broad operating range. However, in order to perform any grade changeover with limited computer memory, the twenty to thirty models should be reduced or re-organized. The problem is how to reduce the number of models while guaranteeing the controllability for all grades. A similar problem was found in the polyethylene polymerization reactor and the GaAs crystallization process.

The integration and coordination of different control schemes is also a problem in the reactor control system. When start-up and shut-down operations are performed for the reactor process, a special control algorithm, which may differ from MPC, might be used. For example, to carry out the start-up operation, a fuzzy-based control system is used by the company working with us on the polyethylene reactor. Because MPC shows superior performance on regulatory and grade changeover control, it is desired to combine the fuzzy-based control system with MPC and to shift the operation from the start-up to regulation without any wind-up and bump.

It may be sated that the difficulties mentioned above are caused by the non-linearity of chemical processes. In academic circles of process control, there has been great interest to develop a practical nonlinear control system. Because of the many successful industrial applications of MPC to systems described by linear models, there are energetic activities for extending the MPC concept to nonlinear control systems. However, nonlinear control theory developed so far is not yet mature enough to offer simple and practical solutions to today's needs for a flexible control system and this situation provides a strong motivation for intelligent controllers.

7. Conclusion

Facing the 21st century, Japanese chemical industries must create a strategy for coping with the current economical situation as well as the changes in demographics and lifestyles. The renewed emphasis on quality improvement is cited as a major factor of resulting in international competition.

Production information integration, hyper-automation, cost reduction and human resource recruitment are progressed as the strategy to deal with the situation. The execution of the strategy needs a practical technology. At present, model based predictive control has attracted strong attention as a control technology. However, MPC is not the panacea in process control. The enthusiasm for development of advanced control and operation techniques based on process understanding is claimed to give simple and practical solutions for more difficult control problems. In addition, future research needs have been elucidated through joint university-industry studies with emphasis on quality modeling, on-line inferential systems, plantwide control and optimization, coordinated control, modeling and control for multirate systems and integration of knowledge-based control with model-based control.

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