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Application of Successive Quadratic Programming to Chemical Process Control

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Abstract

For more economiccal operation of chemical plants, optimal operating conditions are to be set and maintained as far as possible. For this purpose, optimizing control is applied to chemical plants. In this study, a process optimizer composed of a process simulator and an optimization routine using Successive Quadratic Programming as optimization technique is developed and the effect of optimizing control is tested on an example process, and a new process optimization strategy based on modified Jacobian matrix is developed.

1. Introduction

As modern industrial society becomes more competitive, more researches for more economical operation are required in chemical industry. One branch of such researches is to establish more efficient process control systems and operate under optimal conditions as much as possible. So as to establish more efficient control systems much work has been done in the field of control structure synthesis in which control system design and process flowsheet design are considered simultaneously. Once a stable, flexible and reliable control system is constructed, the designation of optimal set-points shouid be followed. However in chemical processes, the flow rates, compositions, temperatures and pressures of feeds fluctuate in some degree. Hence the optimality of initially given operating conditions is broken off and it is necessary to introduce dynamic optimization. But total process of a chemical plant is too large in size and too complex in structure and its modeling equations are highly nonlinear and in general it has large time lag. So, dynamic optimization of a total chemical plant is not only too troublesome but also unnecessary in parctice. Instead of direct application of dynamic optimization, by iterating steady-state optimization with proper time interval, pseudo-dynamic optimization effects can be obtained.

Though an efficient process optimizer is necessary for such purpose, traditional Sequential Modular Approach demands too much computing time. Then, at the beginning of 1980's, with the rapid development of nonlinear programming technique, Simultaneous Modular Approach which converges process flowsheet and process optimization simultaneously appeared and applied to the chemical process design and optimal operation. Within this branch a new optimization strategy was proposed and its performance is now being investigated(1). On the basis of this study, proposed strategy will be expanded into on-line optimization.

In the previous study of on-line optimization, as optimization technique, Nasi et.al.(2) used Conjugate Gradient Method for Acetylene Hydrogenation

Process, Sourander et.al.(3) used Successive Linear Programming for Olefin-cracking Heater in Neste OY's Ethylene Unit and Prett et.al.(4) used Successive Linear Programming for Fluid Catalytic Cracking Unit. And Sofer et.al.(5) reported profit increased case by employing on-line steady-state optimization for hydrocracker column.

In this study a process optimizer composed of a process simulator and optimization routine using Successive Quadratic Programming as optimization method is developed. The effect of on-line steady-state optimization is tested with developed process optimizer for an example process. The values of objective functions under initially fixed optimal point and continually resetted optimal point are compared with each other while the component flow rates of feed stream vary continuously. And as mentioned above for more efficient calculation of process optimization problem, a new optimization strategy is proposed by the modification of Jacobian matrix which is constructed in the traditional optimization strategies.

2. Optimizing control

With the rapid development of computer system, process optimization becomes a large help to process control. Many times a human operator does not or cannot find the best operating policy for a plant which will optimize given objectives. This difficulty is due to the enormous complexity of a typical chemical plant. In such cases we can use the speed and the programmed intelligence of a digital computer to analyze the given process and suggest more reliable policy. Computer control can implement such concepts very well. Computer control is usually classified into two modes; supervisory control and direct digital control (DDC). Direct digital control requires that all the controller action be carried out by the digital computer. Measurements are sent to the computer and compared with given set-points, then the computed control action is transimitted to the actuator. Supervisory control illustrated in Fig. 1 (6) involves resetting the set-point of the local controller according to some control algorithm. Thus the computer control scheme need only supervise and coordinate the actions of the local controllers.

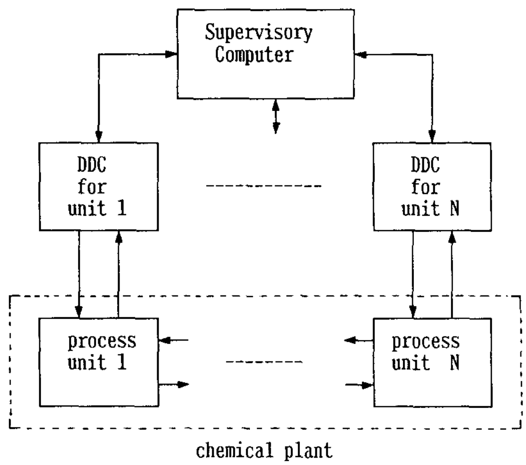

Fig. 1 Supervisory computer control

Nowadays, recently developed efficient process optimization algorithm is involved in the control scheme and this concept is called optimizing control. In optimizing control, with the variation of process system condition, computer calculates the new optimum set-point values and they are transmitted to the controllers. Optimizing control is used extensively today and its future looks even more promising. It is particulary beneficial for large chemical plants where even small improvement in the operating cost are multiplied by large production throughputs. And for the flexible application of optimizing control to chemical process, more efficient optimization strategy is required.

3. Optimization algorithm and the structure of developed process optimizer

When one is faced with a chemical process optimization problem the major difficulty is that this problem is composed of several hundred or several thousand nonlinear equality and inequality constraints. Before process optimizers were developed, a design engineer would usually adjust one or more of the design variables, then simulate the given process and evaluates objective function. Based on these results, he would check the inequality constraints, then readjust design variables and repeat mentioned procedure. However with the developement of nonlinear programming methods, powerful optimizers have appeared and replaced designer's role. Though many nonlinear programming methods are available, the most recent and perhaps the best one is Successive Quadratic Programming method. Wilson(7) long ago proposed an algorithm that approximated the objective function locally by a quadratic function, and the relevant constraints, by linear functions, so that quadratic programming could be used recursively.

Han(8) and Powell(9) developed above scheme into complete algorithm called SQP(Successive Quadratic Programming) by guaranteeing global optimality and superlinear convergence. Westerberg et.al.(10,11) improved this algorithm.

In the developed process optimizer, SQP method is selected as optimization technique and Complementary Pivoting Algorithm is used in solving quadratic programming problem. Fig. 2 illustrates overall calculation scheme of developed process optimizer and Sequential Module Based Approach was implemented in it. In Fig. 2 the loop by dotted line is added when ths process optimizer is used for on-line steady-state optimization. Though Sequential Module Based Approach shows better performance than Sequential Modular Approach, it also requires too much time. So as to improve this feature, much work has been done by Biegler(12), Kisala and Trevino-Rozano(13), etc.. Such researches may be distinguished into two modes: Sequential Module Based Approach and Two-Tier Approach. The characteristics of these two approaches depend on the Jacobian matrix constructed at the third block of Fig. 2 and are represented briefly in Table.1.

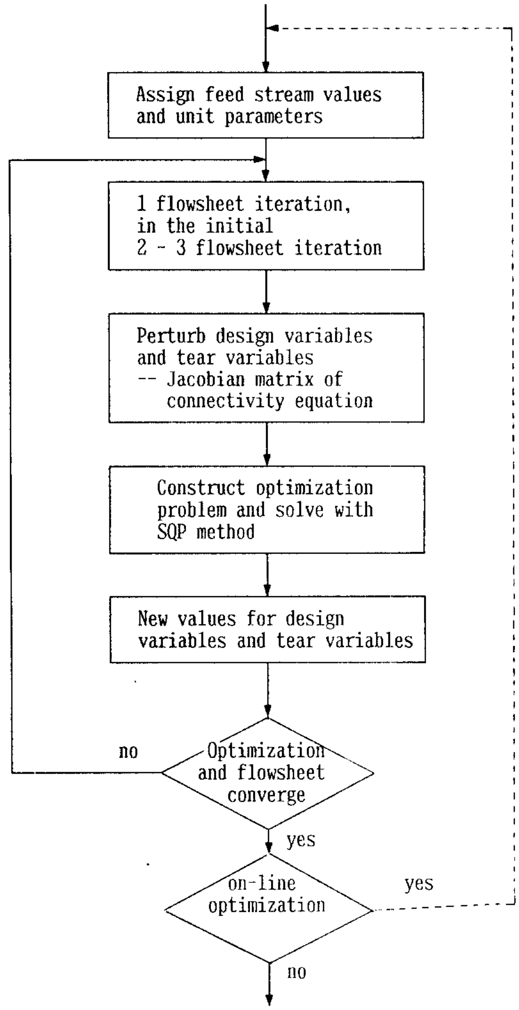

Fig. 2 Schematic calculation scheme of developed process optimizer

On the other hand, a new strategy which is better in performance and convergence is proposed(1). The new strategy developed is based on the facts that precise gradients for decision variables are necessary and gradients with reduced models are accurate enough for flowsheet convergence. Hence Jacobian matrix for process optimization is modified as below in the developed strategy.

Table 1. Comparisons between Sequential Module Based Approach and Two-Tier Approach.

	Sequential Module Based Approach	Two-Tier Approach
Construction of Jacobian matrix	Tear stream connectivity equations and design specification equations vs. Decisign variables and tearing variables	Reduced model equations and design specification equations vs. Decision variables and state variables
Characteristics	Optimal solution is guaranteed Large amount of computation time	Suboptimal solution may be obtained Small amount of computation time
Modifications	Jacobian matrix approximation or Introduction of reduced model for Jacobian matrix calculation when the solution is not near	Restart with Sequential Modular Approach after the solutions based on the reduced model are obtained

$$\left[\begin{array}{c|c} \dfrac{\partial g}{\partial x} & \dfrac{\partial g}{\partial u} \\ \hline \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial u} \end{array}\right]$$

where
g_r : tear stream connectivity equation with reduced model
g_R : tear stream connectivity equation with rigorous model
f : constraints
x state variable
u decision "

Jacobian matrix shown above guarantees both optimality and good performance. And as can be seen in the structure of Jacobian matrix, proposed strategy becomes comparatively more efficient than traditional strategies as the number of tearing variables increases.

4. Example problem

A hypothetical simple flash problem used by Biegler et.al.(14) is selected as an example problem. The process flowsheet is presented as Fig. 3. A light hydrocarbon feed is mixed with recycled bottoms and flahed adiabatically. The vapor is removed as a product, and the liquid split into a bottom product and the recycle, which is pumped back to the feed. Fig. 3 is redrawn as Fig. 4 for the optimization on the developed process optimizer.

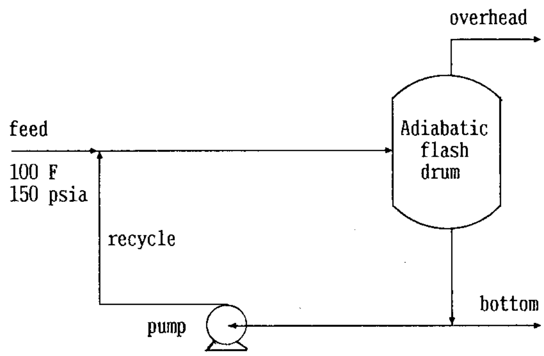

Fig. 3 SImple flash process flowsheet.

Propane	10
1-Butene	15
N-Butane	20
T-2-Butene	20
C-2-Butene	15
Pentane	10

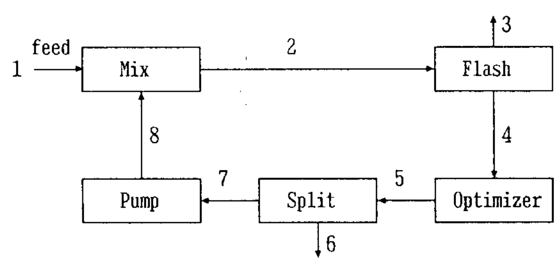

Fig. 4 Flash problem -- calculation structure on POP

In the determination of calculation sequence, optimization routine is included between pump and splitter. Optimization problem is as below.

$$\text{Max} \quad (f_1^2 f_2 - f_1^2 - f_3^3 + f_4 - f_5)$$

$$\text{s.t.} \quad 10 \leq p \leq 50$$
$$0 \leq y_i \leq 100 \quad (i = 1,6)$$
$$0 \leq y_7 \leq 10E7$$

independent variable p, y_i , y_7

where f_i = component flow rate of flash unit vapor stream (bmol/hr)
y_i = component flow rate of stream 5 (bmol/hr)
y_7 = stream enthalpy of stream 5 (btu)
p = pressure of flash unit

In the originaly proposed problem, split ratio of splitter was also an independent variable. But it is proved to be inadequate as an independent variable. So, split ratio is fixed at an arbitrary value 0.7 and only p is designated as an independent variable here.

5. Results and discussion

At first, the example problem was optimized with average component flow rates of the feed stream; average component flow rates appear at Fig. 4. The optimal pressure was 22.27 psia. Then the given process was simulated continuously with the varition of feed stream as Fig. 5 under fixed optimal pressure. As results, variation of the value of objective function is shown in

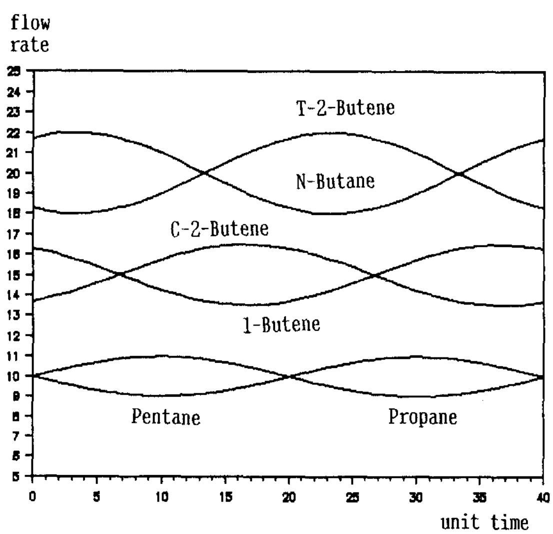

Fig. 5 Variation of feed stream component flow rates.

Fig. 6. The average value of objective function is -0.95635. Next, if f varies more than ±3% arbitrary value, new optimal

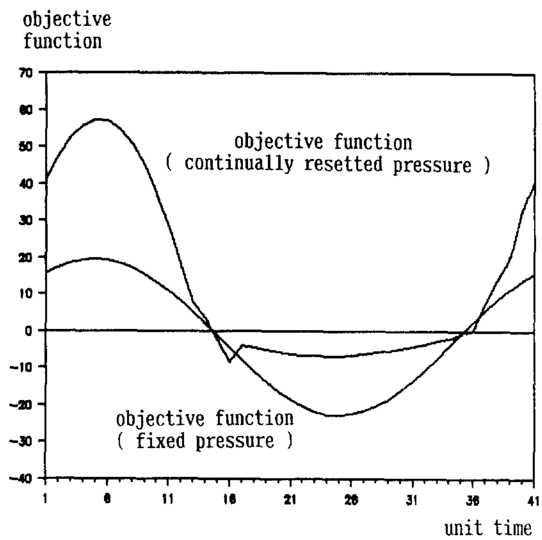

Fig. 6 Variation of the value of objective function.

pressure was assigned for flash unit. The results are shown in Fig. 6 and average value of objective function was 15.153. Fig. 7 represents the variations of optimal pressure of flash unit.

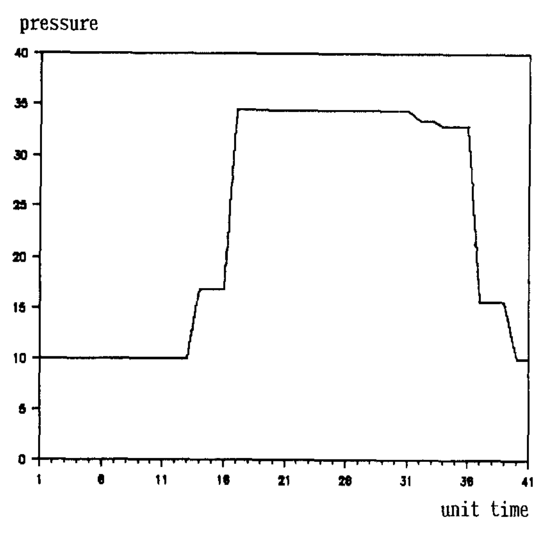

Fig. 7 Variation of optimal pressure.

In this example problem, the given objective function has no economical meaning and is used only for the comparison between above two cases. Under the given objective function, it is easily seen at Fig. 7 that the variation of optimal pressure of flash unit is far larger than that of feed stream component flow rates. Such as like this trend is also prominent at the value of objective function. One of the outstanding feature of chemical process is its large throughputs. Hence as mentioned earlier, even small amount of improvements in operating conditions are invaluable. In this respect obtained results of this example problem are worthy of note.

Developed process optimizer is based on traditional Sequential Module Based Approach and in this example more than 10 STE is needed for one optimization convergence on the average. In some process it would require too much computing time to be applied. For example, on the case of Naphtha Cracking Process, more than 5 hours are required for 1 flowsheet simulation: with MICRO VAX II and ASPEN PLUS. So, it is almost impossible to apply on-line optimization with such optimization strategy. Thus, for the more flexible application of on-line steady-state optimization it will be much beneficial to employ more efficient optimization strategy. On the other hand, the developed strategy requires less amount of computation by about 3 times than the strategy used in the developed process optimizer for the same example process at its initial conditions. Detailed comparisons between the developed optimization strategy and other optimization strategies will be presented after many case studies.

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