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OPTIMIZING CHEMICAL PLANT OPERATION BY MIXED INTEGER PROGRAMMING

Hiroshi Konno
Tokyo Institute of Technology

Hiroaki Sekino
Research Center, Mitsubishi Chemical Industries, Ltd.

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Abstract This paper addresses itself to the maximization of the yield of some chemical process subject to various operational as well as physical constraints. Some of the operational constraints on such factors as the level of flows and the number of flow change are discrete in nature and standard mathematical formulation leads to a medium scale mixed integer programming problem. A typical problem contains 150 integer variables in addition to 150 continuous variables and 200 constraints. A problem of this size may not possibly be solved by the general purpose mixed integer programming code in accordance with our basic requirement, i.e., in less than one minute on 1 MIPS computer.

Thus we introduce a series of relaxation schemes by elaborating the special structure of the problem and reduce the original problem into a set of subproblems, all of which can be solved by standard methods.

We tested this algorithm on a number of real scale problems and always obtained almost optimal solution within 1 minute, whose discrepancy from the true optimum was less than 1% relative to the value of the objective function.

1. Introduction

Let us consider an optimization problem associated with a chemical process depicted in Fig. 1, where some chemical by-product generated while processing main product in plant F is sent to plant A to recover its valuable ingredients. The capacity of plant A is relatively small compared to largely fluctuating input, so that it is temporarily stocked in the intermediate storage S before processed in plant A. The amount in excess of the capacity of the storage S will be burned in plant B.

We naturally want to maximize the amount of flow into plant A or equivalently minimize the amount to be sent to plant B. There are, however, several constraints on the operation of each plant.

First of all, the level of flow into plant A can be adjusted only once a day.

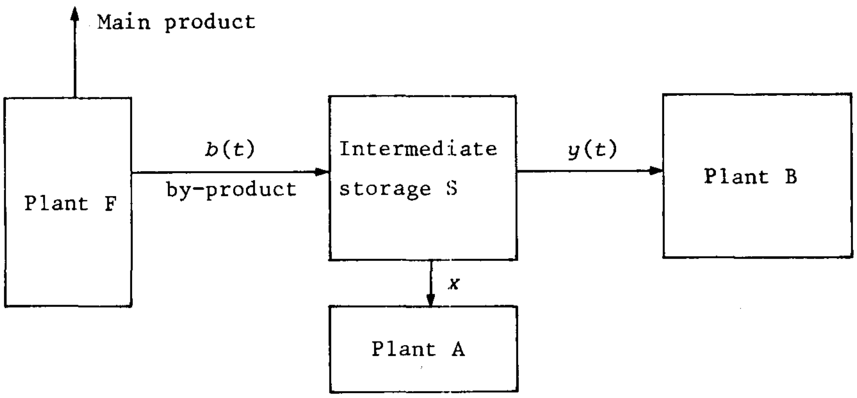

Fig. 1

The level of flow into plant B can be adjusted more frequently, typically as many as ten times every twenty-four hours, but it is preferred to have as few changes as possible primarily because too many changes will put excessive load on the operator. In addition, it must be integer multiple of some positive constant. Also, lower and upper bound constraints are imposed on each variable.

The traditional operation of this system can be described as follows. We set the amount of flow into plant A at the level much lower than the presumably best achievable value to avoid the fatal violation of lower bound constraint of the storage S. According to this scheme, we usually have to

(i) burn much more than necessary

(ii) change the level of flow into plant B intolerably often

which motivated our present effort to optimize the operation using advanced mathematical programming technique.

We will formulate this problem as a mixed integer programming problem in Section 2. A typical discretization of the original continuous time problem leads to a mixed integer linear programming problem consisting of some 150 integer variables and 200 constraints. A problem of this size could not possibly be solved by a general purpose mixed integer programming code within one minute on 1 MIPS computer, which is the crucial requirement imposed on our solution strategy.

We therefore develop a special purpose algorithm in Section 3 where we incorporate a series of relaxations by exploiting the special structure of this problem. As shown in Section 4, our algorithm can generate an almost optimal solution for every input data we examined. It turned out that the difference of the value of the objective function is always less than 1% from that of the true optimum. Also, we could significantly reduce the number of changes of flow into plant B.

There are only a few publications on the applications of mathematical programming techniques to the optimization of chemical process in our country, at least to our knowledge [2,3,5,7].

In particular, we could find almost no published reports on the applications of mixed integer programming. We hope that this paper will call upon a new interest in the applications of mixed integer programming in this field.

2. The Model

Let $b(t)$ be an exogenous function representing the amount of flow into intermediate storage S at time t. Also, let

x : rate of flow into plant A

$y(t)$: rate of flow into plant B at time t

$z(t)$: amount in storage S at time t

The following equation represents the flow balance at storage S

$$(1)\qquad \left.\begin{aligned} &\frac{d}{dt}z(t) = b(t) - x - y(t), \qquad 0 \leqq t \leqq T \\ &z(0) = z_0 \end{aligned}\right\}$$

where T is the planning horizon, usually twenty-four hours. Lower and upper bound constraints are imposed on the variables:

$$(2)\qquad \left.\begin{aligned} &0 \leqq x \leqq x_{\max} \\ &y_{\min} \leqq y(t) \leqq y_{\max}, \quad 0 \leqq t \leqq T \\ &z_{\min} \leqq z(t) \leqq z_{\max}, \quad 0 \leqq t \leqq T \end{aligned}\right\}$$

Also, $y(t)$ should be an integer multiple of positive constant a, i.e.,.

$$(3)\qquad \left.\begin{aligned} &y(t) = w(t)\cdot a\ , \\ &w(t) \text{ is a nonnegative integer for all } t \end{aligned}\right\}$$

Finally $y(t)$ should be a piecewise constant function with at most ten discontinuous points. Our problem is to maximize the yield x subject to constraints described above.

To solve this problem, we discretize time interval of 24 hours into τ minutes subintervals to obtain the following discretized version of equation (1)

$$(4) \qquad x + y_j + \alpha(z_j - z_{j-1}) = b_j, \qquad j=1,\ldots,n$$

where $n = 1440/\tau$, $\alpha = 1/\tau$. Constraints on the number of discontinuities of $y(t)$ can be represented by introducing n zero - one variables as follows:

$$(5) \qquad \left.\begin{array}{ll} y_j - y_{j-1} + mp_j \geqq 0, & j=1,\ldots,n \\ -y_j + y_{j-1} + mp_j \geqq 0, & j=1,\ldots,n \\ \sum_{j=1}^{n} p_j \leqq 10 & \\ p_j \in \{0,\ 1\}, & j=1,\ldots,n \end{array}\right\}$$

where m is a large positive constant. It is easy to see that $p_j = 0$ implies $y_j = y_{j-1}$ whereas $p_j = 1$ implies

$$m \geqq y_j - y_{j-1} \geqq -m$$

which imposes no restriction on $y_j - y_{j-1}$ when m is large enough, so that constraints (5) judiciously represent our restriction on the number of discontinuities.

Our problem can now be written as follows:

$$(6) \qquad \left|\begin{array}{lll} \text{maximize} & x & \\ \text{subject to} & x + y_j + \alpha(z_j - z_{j-1}) = b_j, & j=1,\ldots,n \\ & 0 \leqq x \leqq x_{\max} & \\ & y_{\min} \leqq y_j \leqq y_{\max}, & j=1,\ldots,n \\ & z_{\min} \leqq z_j \leqq z_{\max}, & j=1,\ldots,n \\ & y_j = w_j \cdot a, & j=1,\ldots,n \\ & w_j \geqq 0, \text{ integer}, & j=1,\ldots,n \\ & y_j - y_{j-1} + mp_j \geqq 0, & j=1,\ldots,n \\ & -y_j + y_{j-1} + mp_j \geqq 0, & j=1,\ldots,n \\ & \sum_{j=1}^{n} p_j \leqq 10 & \\ & p_j \in \{0,\ 1\}, & j=1,\ldots,n \end{array}\right.$$

Typically when τ=20(minutes) this problem contains about 150 integer variables in addition to 150 continuous variables. Also it has about 200 constraints other than lower and upper bound constraints on the variables. We are requested to supply an optimal yield x^* and associated operation scheme within one minute after the input data $b(t)$ is provided from the factory every morning.

3. Algorithmic Strategy

The problem formulated in Section 2 is a medium scale mixed integer programming problem which could not be solved in one minute on 1 MIPS computer by the state-of-the-art general mixed integer programming code. We are thus forced to devise an approximation of the model and a special purpose algorithm to solve a resulting approximate problem.

We will describe here a very successful relaxation strategy consisting of the following four steps.

[Step 1]

We will first relax the complicating constraints related to the number of discontinuities of y_j's and solve the resulting linear programming problem:

$$(7)\qquad \left|\begin{array}{lll} \text{maximize} & x & \\ \text{subject to} & x + y_j + \alpha(z_j - z_{j-1}) = b_j, & j=1,\dots,n \\ & 0 \leqq x \leqq x_{\max} & \\ & y_{\min} \leqq y_j \leqq y_{\max}, & j=1,\dots,n \\ & z_{\min} \leqq z_j \leqq z_{\max}, & j=1,\dots,n \end{array}\right.$$

Let $\bar{x}$, $\bar{y}_j$, $\bar{z}_j$, $j=1,\dots,n$ be an optimal solution of this problem. Obviously $\bar{x}$ gives an upper bound of the optimal solution x^* of (6), i.e.,

$$(8)\qquad \bar{x} \geqq x^*$$

[Step 2]

We are slmost done if the number of discontinuities associated with $\bar{y}_j$'s are less than 10. It is, however, an exceptional case and we try to reduce the number of discontinuities by solving another subproblem:

$$(9)\quad \begin{array}{lll} \text{minimize} & \sum_{j=1}^{n} |y_j - y_{j-1}| & \\ \text{subject to} & y_j + \alpha(z_j - z_{j-1}) = b_j - \bar{x}, & j=1,\dots,n \\ & y_{\min} \leqq y_j \leqq y_{\max}, & j=1,\dots,n \\ & z_{\min} \leqq z_j \leqq z_{\max}, & j=1,\dots,n \end{array}$$

It is straightforward to see that this problem has an optimal solution $\hat{y}_j$, $\hat{z}_j$, $j=1,\dots,n$, which can be obtained by solving an equivalent linear programming problem:

$$(10)\quad \begin{array}{lll} \text{minimize} & \sum_{j=1}^{n} (v_j^+ + v_j^-) & \\ \text{subject to} & y_j + \alpha(z_j - z_{j-1}) = b_j - \bar{x}, & j=1,\dots,n \\ & y_{\min} \leqq y_j \leqq y_{\max}, & j=1,\dots,n \\ & z_{\min} \leqq z_j \leqq z_{\max}, & j=1,\dots,n \\ & y_j - y_{j-1} - v_j^+ + v_j^- = 0, & j=1,\dots,n \\ & v_j^+ \geqq 0,\ v_j^- \geqq 0, & j=1,\dots,n \end{array}$$

[Step 3]

Since we want to have as few discontinuities as possible, we will try to further reduce it. Let k be the number of discontinuous points associated with $\hat{y}_j$, $j=1,\dots,n$ and let $j_1, j_2,\dots,j_k$ be the time at which the jump takes place. We will introduce k variables $\eta_1, \eta_2,\dots,\eta_k$, one for each interval on which y_j's are constant and rewrite the constraint of problem using these k variables instead of y_j's. (See Fig. 2)

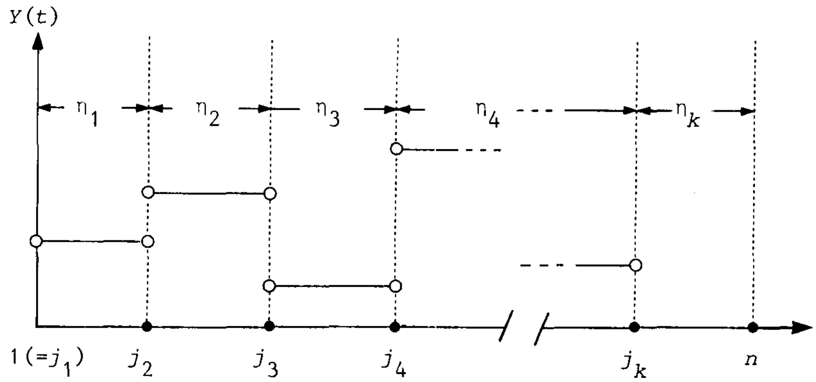

Fig. 2

We thus solve a sequence of k linear programs LP(ℓ) for $\ell=1,\ldots,k$:

$$\text{(11)}\qquad \mathrm{LP}(\ell)\left|\begin{array}{lll} \text{minimize} & |\eta_\ell - \eta_{\ell-1}| & \\ \text{subject to} & \eta_i + \alpha(z_j - z_{j-1}) = b_j - \bar{x}, & \\ & \quad j = j_i, j_i+1, \ldots, j_{i+1}-1, & i=1,\ldots,k \\ & y_{\min} \leqq \eta_i \leqq y_{\max}, & i=1,\ldots,k \\ & z_{\min} \leqq z_j \leqq z_{\max}, & j=1,\ldots,n \\ & \eta_s - \eta_{s-1} = 0, & s \in J_\ell \end{array}\right.$$

where $J_1=\phi$ and J_ℓ is recursively defined as follows:

$$J_{\ell+1} = \begin{cases} J_\ell \cup \{\ell\} & \text{if the optimal value of the objective function of LP}(\ell) \text{ is zero} \\ J_\ell & \text{otherwise} \end{cases}$$

If the resulting number of discontinuities is greater than 10, we have to gradually decrease the level of x from its best achievable value $\bar{x}$ and solve (9) again until this requirement is satisfied (Fortunately, this routine was not activated for all test problems.)

Let $j_1, j_2, \ldots, j_p$ be points of discontinuities of y_j's, where $p \leqq 10$.

[Step 4]

Solve the following mixed integer program generated from (6) by fixing p time points $j_1,\ldots,j_p$ at which jump of y_j is possible.

$$\text{(12)}\qquad \left|\begin{array}{lll} \text{maximize} & x & \\ \text{subject to} & x + y_s + \alpha(z_j - z_{j-1}) = b_j & \\ & j_s + 1 \leqq j \leqq j_{s+1}, & s=1,\ldots,p \\ & 0 \leqq x \leqq x_{\max} & \\ & y_{\min} \leqq y_s \leqq y_{\max}, & s=1,\ldots,p \\ & z_{\min} \leqq z_j \leqq z_{\max}, & j=1,\ldots,n \\ & y_s = \text{integer multiple of } a, & s=1,\ldots,p \end{array}\right.$$

This problem contains less than ten integer variables y_s, $s=1,\ldots,p$ so that it can be solved by standard branch and bound technique. We will employ the optimal solution $(\tilde{x}, \tilde{y}_1,\ldots,\tilde{y}_p, \tilde{z}_1,\ldots,\tilde{z}_n)$ of (12) as our approximate optimal solution of (6) by nothing that it is a feasible solution of (6).

Fig. 3 shows the flow chart of our solution strategy. Note that each subproblem (7), (9) and (12) are significantly easier than (6).

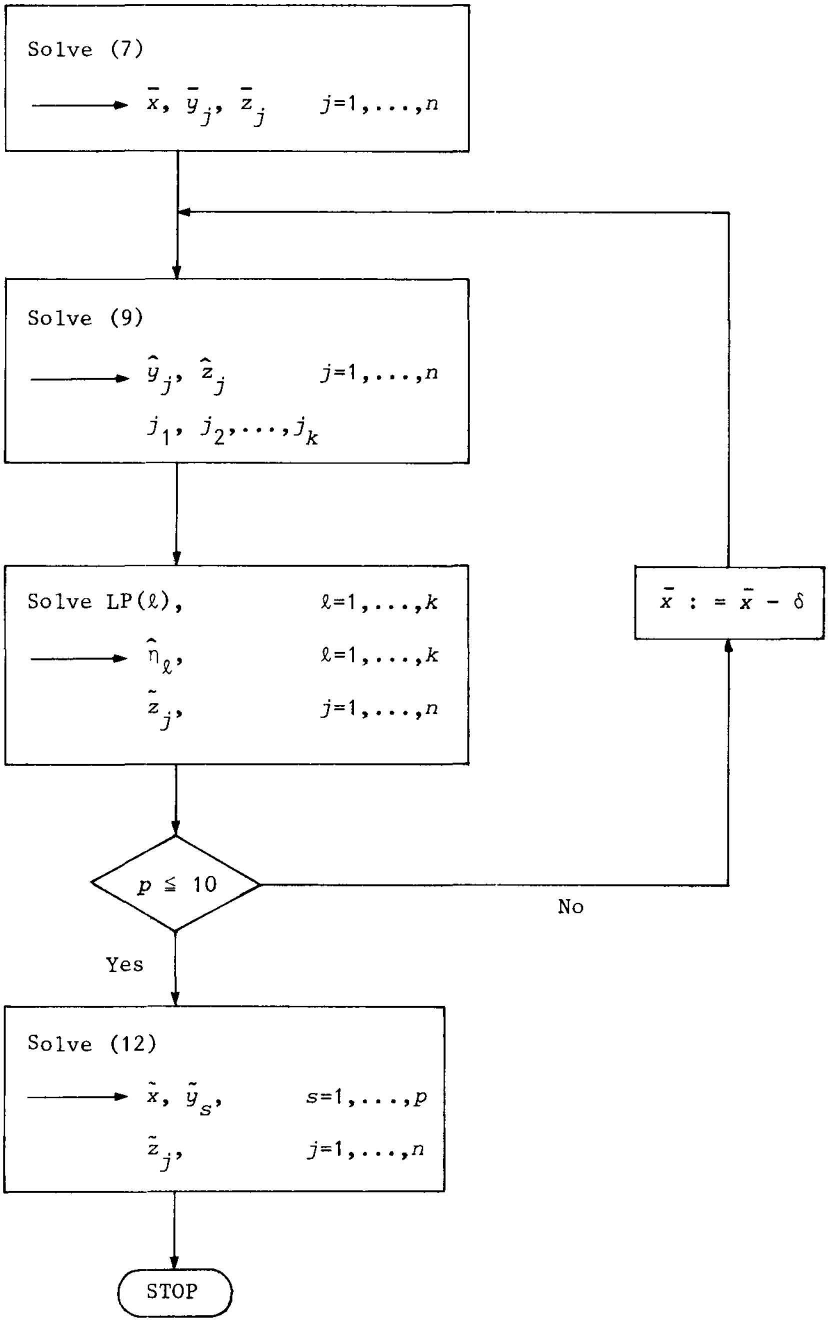

Fig. 3 Strategy for Solving (6)

4. Computational Results

We first compared our solution strategy with the traditional method which is based upon the experience and intuition of the operator in charge of this system. Table 1 summarizes the result where τ=60(minutes) in all four cases.

Table 1

	Attained yield x (ℓ/hr)		Number of jumps of y_j's	
	Traditional method	New method	Traditional method	New method
Case A	154.0	170.8	5	2
Case B	152.0	164.4	7	2
Case C	162.8	171.6	6	2
Case D	164.8	181.7	9	2

This table shows that our method always generates a solution whose yield is about 10% better than the traditional method. Also the number of jumps is remarkably less.

We next applied our method to the typical input data depicted in Fig. 4.1 where τ=20(minutes). Fig. 4.1 shows the optimal solution of (7) and Fig. 4.2 shows the optimal solution of (9). Note that the number of discontinuities of $y(t)$ dropped from 12 in Fig. 4.1 to 3 in Fig. 4.2. Fig. 4.3 shows the solution after solving k linear programs LP(ℓ), $\ell=1,\dots,k$ where the number of discontinuities decreased even further. Fig. 4.4 shows the optimal solution of (12) where $\tilde{x}$ is greater than $0.99\bar{x}$. We thus obtained a feasible solution of (6) in which $\tilde{x}$ satisfies

$$x^* \geqq \tilde{x} \geqq 0.99x^*$$

by noting (8).

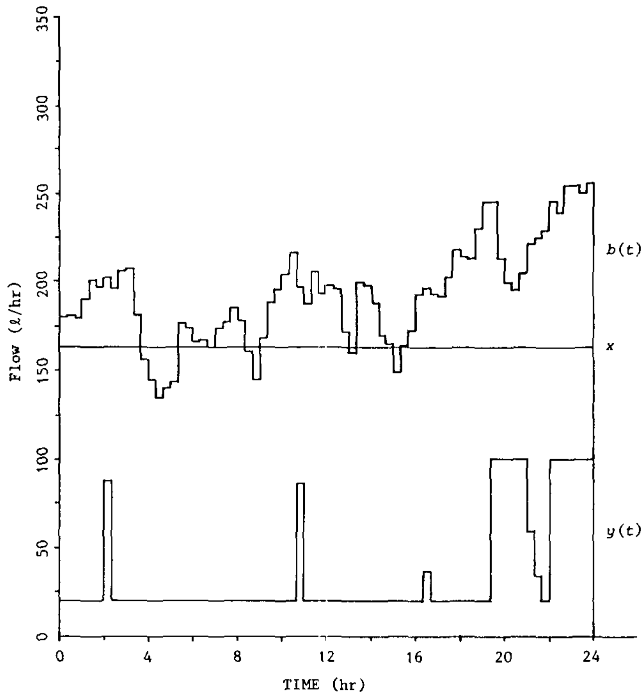

Fig. 4.1 (a)

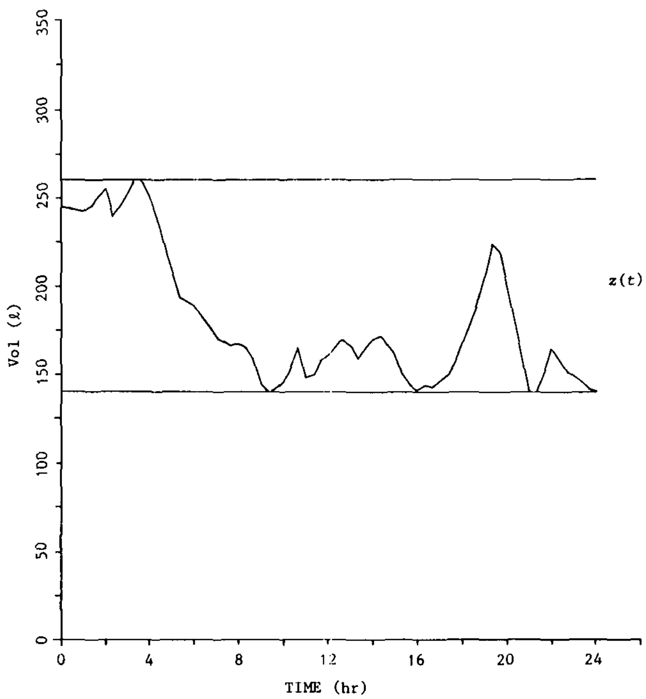

Fig. 4.1 (b)

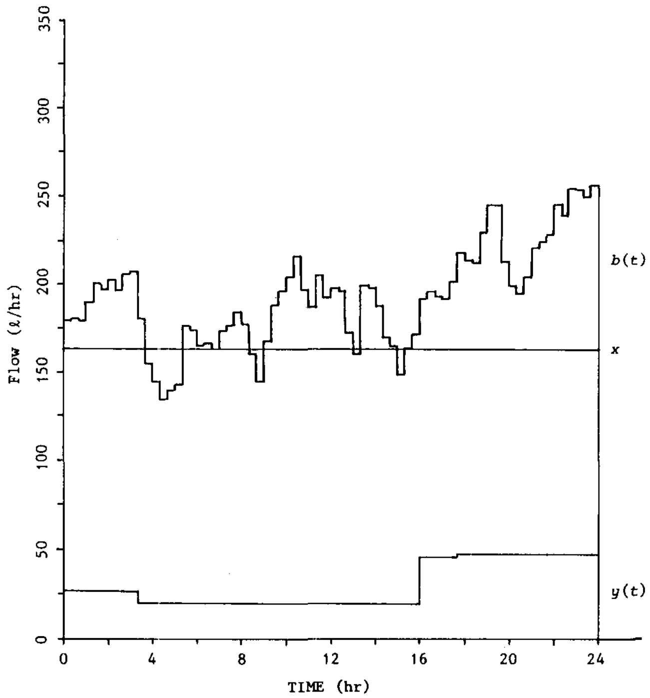

Fig. 4.2 (a)

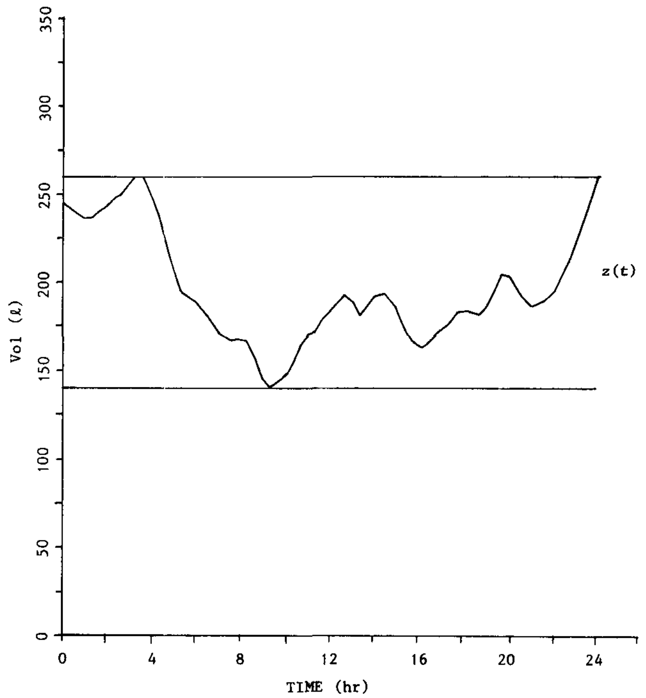

Fig. 4.2 (b)

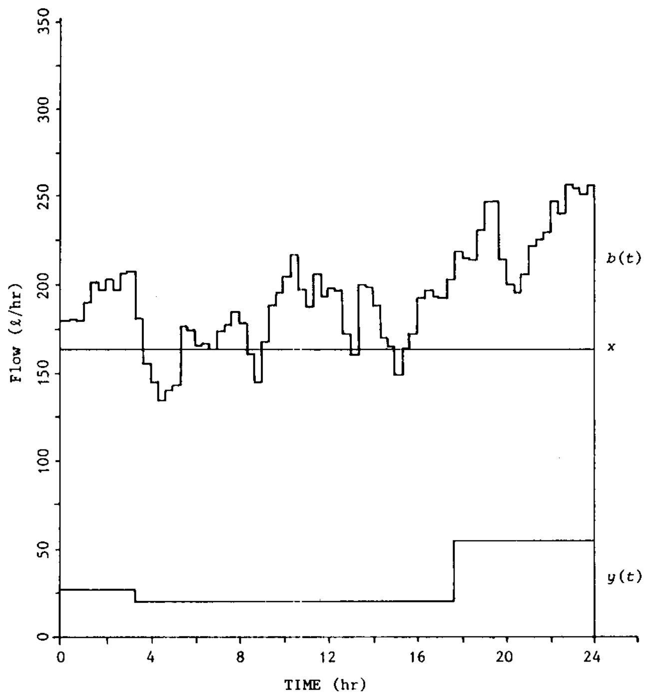

Fig. 4.3 (a)

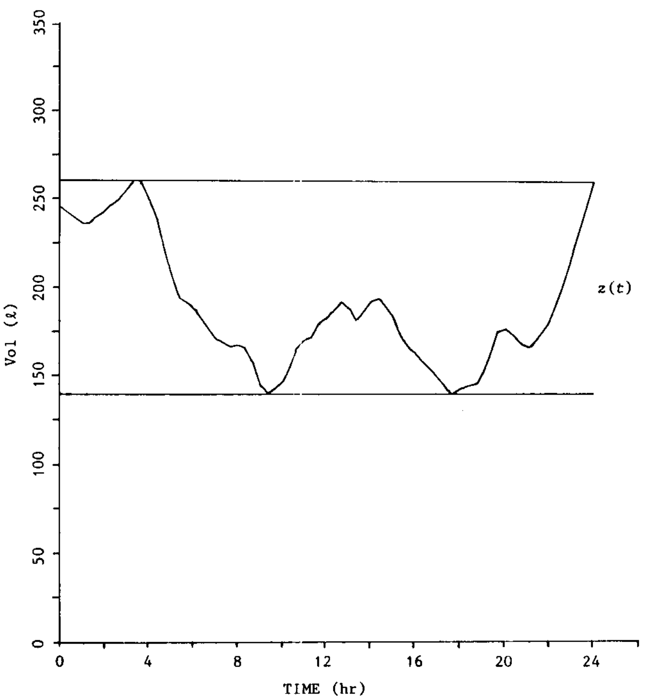

Fig. 4.3 (b)

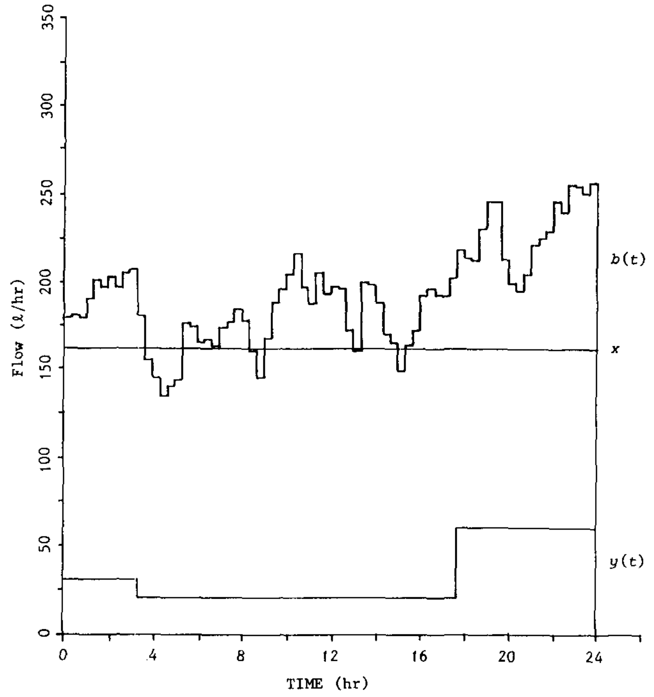

Fig. 4.4 (a)

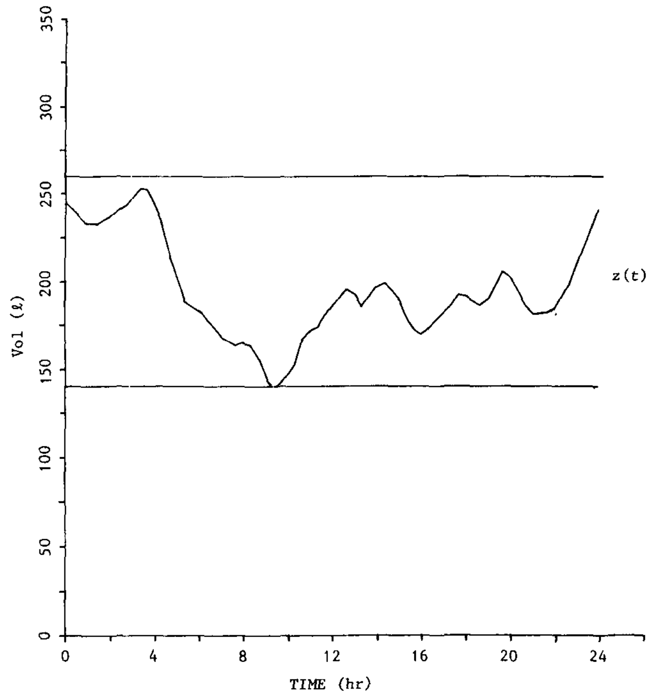

Fig. 4.4 (b)

Table 2 shows some of the more important constants used in our computation. Table 3 shows the value of $\bar{x}$ and $\tilde{x}$ for four different input data. We observe from this that the difference from x^* are less than 1%. Also, we observe from Table 4 that the number of discontinuities is less than 3 in each case. (See in particular a remarkable success in Case 4.)

Every result shows the validity of our solution strategy. It should be emphasized that these remarkable success was not expected at all before we started this study since τ=20(minutes) problem has been too complicated to obtain a reasonably good operation scheme by traditional approach based on experience and intuition.

Table 2. Physical Constants

x_{max}	y_{min}	y_{max}	a	z_{min}	z_{max}	τ
200 (ℓ/hr)	40 (ℓ/hr)	100 (ℓ/hr)	5 (ℓ/hr)	140 (ℓ)	260 (ℓ)	20 (min)

Table 3. Attained Yields

	$\bar{x}$(ℓ/hr)	$\tilde{x}$(ℓ/hr)	$\tilde{x}/\bar{x}$
Case 1	187.4	186.8	0.997
Case 2	172.0	171.7	0.998
Case 3	162.8	161.5	0.993
Case 4	155.9	154.7	0.992

Table 4. Number of Flow Change

	Step 1	Step 2	Step 3
Case 1	8	3	3
Case 2	5	4	2
Case 3	12	4	3
Case 4	14	3	3

Finally, Table 5 shows the amount of time required to obtain this solution, which successfully meets the computational requirements.

We expect from these results that this method can solve an even larger problem with smaller τ(say 5 minutes) or longer planning horizon (say 1 week) by

(i) using more elaborate implementation technique instead of the rudimentary upper bounded simplex method currently in use

(ii) skipping the most time consuming Step 3 and instead using the best least square approximation procedure [6] of a piecewise constant function by another piecewise constant function with a fixed number of jumps.

Table 5. CPU Time (seconds)

	Step 1	Step 2	Step 3*	Step 4
Case 1	10	8	≦ 30	3.7
Case 2	9	20	≦ 36	3.8
Case 3	10	10	≦ 40	3.5
Case 4	4	12	≦ 32	9.7

Step 1 ∿ 3 FACOM M 180 II AD
(hand-made simplex routine)
Step 4 IBM 3081 MPSX/MIP
(These values are changed to M 180 II AD at the rate of MIPS)

* Include overhead jobs. Real execution time is considerably less.

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Hiroaki SEKINO: Mathematical System
Laboratory, Research Center,
Mitsubishi Chemical Industries, Ltd.
1000, Kamoshida, Midori-ku, Yokohama,
Japan.