# Optimal Design of Batch-Storage Network with Recycle Streams

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An effective methodology is reported for determining the optimal capacity (lot size) of batch processing and storage networks which include material recycle or reprocessing streams. It is assumed that any given storage unit can store one material type which can be purchased from suppliers, internally produced, and internally consumed and/or sold to customers. It is further assumed that a storage unit is connected to all processing stages that use or produce the material to which that storage unit is dedicated. Each processing stage transforms a set of feedstock materials or intermediates into a set of products with constant conversion factors. The objective for optimization is to minimize the total cost composed of raw material procurement, setup, and inventory holding costs, as well as the capital costs of processing stages and storage units. A novel production and inventory analysis formulation, the PSW model, provides useful expressions for the upper/lower bounds and average level of the storage inventory holdup. The expressions for the Kuhn-Tucker conditions of the optimization problem can be reduced to two subproblems. The first yields analytical solutions for determining batch sizes, while the second is a separable concave minimization network flow subproblem whose solution yields the average material flow rates through the networks. For the special case in which the number of storage units is equal to the number of process stages and raw materials storage units, a complete analytical solution for average flow rates can be derived.

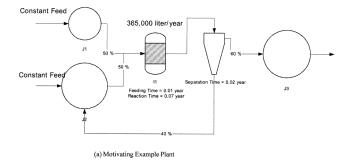
## Introduction

The purpose of this study is to suggest an effective methodology to determine the optimal capacity (lot-size) of general batch-storage network including recycling streams. We already have developed the compact analytical solution of the optimal lot sizing of multiproduct, sequential multistage production and inventory system with serially and parallel interlinked storage units and processes (Yi and Reklaitis, 2002). In this study, we enlarge the network connection struc-

ture of the storage units and the processes to the most general form. We assume that any storage unit can be connected to any process as feedstock and/or product. A practical advantage of this study over our previous work exists in that we can deal with the network structure involving nonsequential recycling streams, which is very popular in chemical processes. In spite of general presentation, analytical solution is still available as a special case.

Recycle streams are naturally required in chemical processes involving reversible exothermic reactions, consecutive reactions  $(A \rightarrow B \rightarrow C)$  with the intermediate B as the de-

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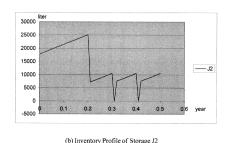


Figure 1. Motivating example process with recycle stream.

sired product, solvent extraction, and wastewater treatment. Recycle streams significantly increase capital and energy costs (Luyben, 2000). The existence of a single recycle stream increases the iteration times of process simulation by more than a dozen. Consider a simple example plant with a recycle stream in Figure 1a. We assume that the feed and product streams are continuous and the process operates batchwise, for simplicity. The inventory holdup where the recycle stream is connected is very complicated, as shown in Figure 1b. The inventory level of feed materials should not be depleted for the proper operation of the batch process. It would be nontrivial work to find a feasible and minimum storage size for the given input and output noncontinuous flows. Moreover, determining the optimal capacity of all equipments and stream flows involving recycle streams without depletion of the storage materials will be a very difficult task. Most real plant design problems involve multiple processes and storage units in serial and/or parallel connections with forward and/or backward flows. Each process consumes a fixed composition of multiple feed materials and produces a fixed yield of multiple products. Each process unit requires a time delay of material flow. Every construction and operation of the process and storage units are followed by several cost factors such as capital cost, setup cost, inventory holding cost, and so on. It would be a challenging work if a unified general model could be found to accommodate all of such design concerns.

Yi and Reklaitis (2000) suggested a novel production and inventory analysis method called periodic square wave (PSW) and applied it to the optimal design of a parallel batch-storage system. They extended the plant structure to the sequential multistage batch-storage network in Yi and Reklaitis (2002). The PSW model is suitable to describe the periodic material flow of a highly interlinked batch-storage system. The

application of it is not limited to the sequential multistage network. In this article, we will apply the PSW model to the nonsequential network involving arbitrary recycling flows. We address an arbitrary circuit with simplified batch processes and storage units. We will focus on obtaining a compact set of analytical solutions. In order to obtain the analytical solution, we assume that all operations are periodical with unknown cycle times. An analytic solution is very useful at the preliminary conceptual design stage, because in the early stages of plant design, detailed information is not yet available. Thus, a rigorous detailed model may be of limited value. At the early plant design stage, it is common that the managerial or strategic decisions are changed due to uncertain market information. Consequently, the subsequent design work requires repeated revision. In this situation, a simple analytic solution has great advantages in responding to a very diverse range of managerial decisions.

The subsequent presentation will proceed as follows. We will introduce the notation for the nonsequential network structure. We assume that all storage units can be connected to all processes that consume or produce those materials to which the storage units are dedicated. One storage unit stores one material which can be purchased from suppliers, internally produced, internally consumed, and/or sold to consumers. The processes transform a set of feedstock materials into another set of products with constant conversion factors. The objective function of optimization is minimizing the total cost composed of raw material purchase, setup, and inventory holding costs, as well as the capital costs of constructing processes and storage units. The PSW model provides useful expressions for the upper/lower bounds and average level of the storage inventory holdup. The Kuhn-Tucker solution to the given optimization problem gives analytic solutions for determining batch sizes and a separable concave minimization network flow problem for determining the average material flow rates through processes and storage units. A special case of analytic solution for the average flow rates exists in that the number of storage units is equal to the number of processes and raw material storage units. An illustrative example will show the effectiveness of our approach.

## **Definition of Parameters and Variables**

A chemical plant, which converts raw materials into final products through multiple physicochemical processing steps, is composed of a set of storage units (J) and a set of batch processes (I), as shown in Figure 2. The circle  $(j \in J)$  in the figure represents a storage unit, the square  $(i \in I)$  represents

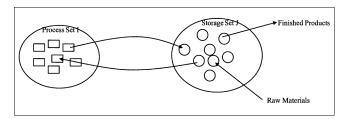


Figure 2. General structure of batch-storage networkprocess and storage sets.

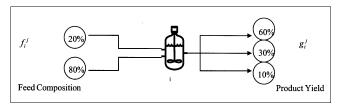


Figure 3. Feedstock composition and product yield of a process.

a batch process, and the arrows represent the material flows. Each process requires multiple feedstock materials of fixed composition  $(f_i^j)$  and produces multiple products with fixed product yield  $(g_i^j)$ , as shown in Figure 3. Note that storage index j is superscript and process index i is subscript. If there is no material flow between a storage unit and a process unit, the corresponding feedstock composition or product yield value is zero. Each storage unit is dedicated to one material. Multiple storage units that store the same material are considered as one storage unit. Each storage is involved with four types of material movement, purchasing from suppliers  $(k \in K(j))$ , shipping to consumers  $(m \in M(j))$ , feeding to processes, and producing from processes, as shown in Figure 4. Note that the sets of suppliers K(j) or customers M(j) are storage dependent. Note also that the stage index n in Yi and Reklaitis (2002) is not necessary any more because the existence of arbitrary recycling streams does not allow identifying the stage sequence. The material flow from process to storage (or from storage to process) is represented by the PSW model, as shown in Figure 5 in Yi and Reklaitis (2002). The material flow representation of the PSW model is composed of four variables: batch size  $B_i$ , cycle time  $\omega_i$ , storage operation time fraction  $x_i^{\text{in}}$  (or  $x_i^{\text{out}}$ ), and startup time  $t_i^{\text{in}}$  (or  $t_i^{\text{out}}$ ). The storage operation time fraction  $x_i^{\text{in}}$  (or  $x_i^{\text{out}}$ ) is the fraction of the time of material movement to (or from) the process over cycle time. The startup time  $t_i^{\text{in}}$  (or  $t_i^{\text{out}}$ ) is the first time at which the first batch is fed into (or discharged from) the process. The feedstock flows from predecessor storages and the product flows to successor storages are, of course, not independent. One production cycle of the batch process is composed of feeding time, processing time, and discharging time. In reality, there may exist sequences of feedstock feeding operations or product discharging operations, and the sequences depend upon material movement system design such as pumping and piping network. There-

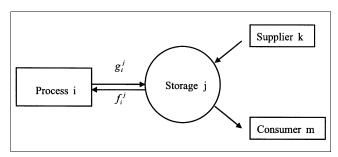


Figure 4. Incoming and outgoing material flows of a storage unit.

fore, the material movement times may not be the same even within a particular stage, in general. However, at the early design stage, such information is not available because the material movement facilities are not designed yet. As far as the design of a material movement system does not significantly influence the process and/or storage size, we, thus, assume that the feedstock feeding operations to the process (or the product discharging operations from the process) occur at the same time and their storage operation time fractions are the same among feeding or discharging flows. That is, the superscript *j* is not necessary to discriminate storage units in the  $x_i^{\text{in}}$  (or  $x_i^{\text{out}}$ ) and  $t_i^{\text{in}}$  (or  $t_i^{\text{out}}$ ). The material flow of raw material purchase is represented by order size  $B_k^j$ , cycle time  $\omega_k^i$ , storage operation time fraction  $x_k^i$ , and startup time  $t_k^j$ . All storage operation time fractions will be considered as parameters, whereas the others will be the design variables as used in this study. The material flow of finished product sales is represented by  $B_m^j$ ,  $\omega_m^j$ ,  $x_m^j$ ,  $t_m^j$  in the same way. The arbitrary periodic function of finished product demand forecast can be represented by the sum of periodic square wave functions with known values of  $B_m^j$ ,  $\omega_m^j$ ,  $x_m^j$ ,  $t_m^j$ (Yi and Reklaitis, 2000).

# **Nonlinear Optimization Model of Plant Design**

From the fact that one production cycle in a process is composed of feedstock feeding time  $(x_i^{\text{in}}\omega_i)$ , processing time,  $([1-x_i^{\text{in}}-x_i^{\text{out}}]\omega_i)$ , and product discharging time  $(x_i^{\text{out}}\omega_i)$ , there exists the following timing relationship between the startup time of feedstock streams and the startup time of product streams

$$t_i^{\text{out}} = t_i^{\text{in}} + \omega_i (1 - x_i^{\text{out}}) \tag{1}$$

Let  $D_i$  be the average material flow rate through process i, which is batch size  $B_i$  divided by cycle time  $\omega_i$ . The average material flows of raw material purchase from suppliers and finished product shipping to consumers are denoted by  $D_k^j$ ,  $D_m^j$ , respectively, where  $D_k^j = B_k^j/\omega_k^j$ ,  $D_m^j = B_m^j/\omega_m^j$ . The overall material balance around a storage unit results in the following relationships

$$\sum_{i=1}^{|I|} g_i^j D_i + \sum_{k=1}^{|K(j)|} D_k^j = \sum_{i=1}^{|I|} f_i^j D_i + \sum_{m=1}^{|M(j)|} D_m^j$$
 (2)

Suppose that the initial inventory of storage j is denoted by  $V^j(0)$  and the inventory holdup of storage j at time t is denoted by  $V^j(t)$ . The inventory holdup can be calculated by the difference between the incoming material flows from supply processes and the outgoing material flows into consumption processes. Special properties of the periodic square wave function are required to integrate the detail material balance equation, as can be seen in the Appendix in Yi and Reklaitis (2002). A storage unit is connected to the incoming flows from suppliers and processes and the outgoing flows into consumers and processes. The resulting inventory holdup

function for a storage unit is

$$V^{j}(t) = V^{j}(0)$$

$$+ \sum_{k=1}^{|K(j)|} B_{k}^{j} \left[ \operatorname{int} \left[ \frac{t - t_{k}^{j}}{\omega_{k}^{j}} \right] + \operatorname{min} \left\{ 1, \frac{1}{x_{k}^{j}} \operatorname{res} \left[ \frac{t - t_{k}^{j}}{\omega_{k}^{j}} \right] \right\} \right]$$

$$+ \sum_{i=1}^{|I|} \left( g_{i}^{j} B_{i} \right) \left[ \operatorname{int} \left[ \frac{t - t_{i}^{\text{out}}}{\omega_{i}} \right] + \operatorname{min} \left\{ 1, \frac{1}{x_{i}^{\text{out}}} \operatorname{res} \left[ \frac{t - t_{i}^{\text{out}}}{\omega_{i}} \right] \right\} \right]$$

$$- \sum_{m=1}^{|M(j)|} B_{m}^{j} \left[ \operatorname{int} \left[ \frac{t - t_{m}^{j}}{\omega_{m}^{j}} \right] + \operatorname{min} \left\{ 1, \frac{1}{x_{m}^{j}} \operatorname{res} \left[ \frac{t - t_{m}^{j}}{\omega_{m}^{j}} \right] \right\} \right]$$

$$- \sum_{i=1}^{|I|} \left( f_{i}^{j} B_{i} \right) \left[ \operatorname{int} \left[ \frac{t - t_{i}^{\text{in}}}{\omega_{i}} \right] + \operatorname{min} \left\{ 1, \frac{1}{x_{i}^{\text{in}}} \operatorname{res} \left[ \frac{t - t_{i}^{\text{in}}}{\omega_{i}} \right] \right\} \right]$$

$$(3)$$

The upper bound of the inventory holdup, the lower bound of the inventory holdup, and the average inventory holdup of Eq. 3 are calculated by using the properties of the flow accumulation function (Yi and Reklaitis, 2002)

$$\overline{V}^{j} = V^{j}(0) + \sum_{k=1}^{|K(j)|} \left(1 - x_{k}^{j}\right) D_{k}^{j} \omega_{k}^{j} - \sum_{k=1}^{|K(j)|} D_{k}^{j} t_{k}^{j} + \sum_{i=1}^{|I|} \left(1 - x_{i}^{\text{out}}\right) g_{i}^{j} D_{i} \omega_{i} - \sum_{i=1}^{|I|} g_{i}^{j} D_{i} t_{i}^{\text{out}} + \sum_{i=1}^{|I|} f_{i}^{j} D_{i} t_{i}^{\text{in}} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right) (4)$$

$$\underline{V}^{j} = V^{j}(0) - \sum_{k=1}^{|K(j)|} D_{k}^{j} t_{k}^{j} - \sum_{i=1}^{|I|} g_{i}^{j} D_{i} t_{i}^{\text{out}} - \sum_{i=1}^{|I|} f_{i}^{j} D_{i} t_{i}^{\text{in}} - \sum_{i=1}^{|M(j)|} \left(1 - x_{i}^{\text{in}}\right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right) (5)$$

$$\overline{V}^{j} = V^{j}(0) + \sum_{k=1}^{|K(j)|} \frac{\left(1 - x_{k}^{j}\right)}{2} D_{k}^{j} \omega_{k}^{j} - \sum_{k=1}^{|K(j)|} D_{k}^{j} t_{k}^{j} + \sum_{i=1}^{|I|} \frac{\left(1 - x_{i}^{\text{out}}\right)}{2} g_{i}^{j} D_{i} \omega_{i} - \sum_{i=1}^{|I|} g_{i}^{j} D_{i} t_{i}^{\text{out}} - \sum_{i=1}^{|I|} \frac{\left(1 - x_{i}^{\text{in}}\right)}{2} D_{m}^{j} \omega_{m}^{j} + \sum_{i=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right) (6)$$

Equation 4 will be used to predict storage size. Equation 5 will be used for no depletion constraint. Equation 6 will be used to calculate inventory holding cost.

The purchasing setup cost of raw material j is denoted by  $A_k^j$  \$/order and the setup cost of process i is denoted by  $A_i$ 

\$/batch. The annual inventory holding cost of storage j is denoted by  $H^{j}$  \$/year/L. The annual capital cost of process construction and licensing cannot be ignored in the chemical process industries. In general cases, capital cost is proportional to some power of process capacity. The typical value of exponent ranges from 0.3 to 1.2 (Peters and Timmerhaus, 1980). In this article, we will assume that capital cost is proportional to process capacity in order to permit an analytical solution. Suppose that  $a_k^i$  (\$/year/L) is the annual capital cost of purchasing facility for raw material j,  $a_i$  (\$/year/L) is the annual capital cost of process i and  $b^{j}$  (\$/year/L) is the annual capital cost of storage unit j. Assume that raw material cost is proportional to the quantity and the purchasing price of raw material j from k supplier is  $P_k^j$  \$/L. Note that, without further complexity, the functionality of the raw material cost with respect to the quantity can be elaborated to any separable concave function by considering the economies of scale. The objective function for the design of the batch-storage network is to minimize the total cost consisting of the raw material procurement cost, the setup cost of processes, the inventory holding cost of storage units, and the capital cost of processes and storage units

$$TC = \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \left[ \frac{A_k^j}{\omega_k^j} + a_k^j D_k^j \omega_k^j \right] + \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \left[ P_k^j D_k^j \right]$$

$$+ \sum_{i=1}^{|J|} \left[ \frac{A_i}{\omega_i} + a_i D_i \omega_i \right] + \sum_{j=1}^{|J|} \left[ H^j \overline{V}^j + b^j \overline{\overline{V}}^j \right]$$
 (7)

Without loss of generality, storage size will be determined by the upper bound of inventory holdup  $V^j$ . Therefore, Eq. 4 is the expression for storage capacity. The independent variables are selected to be cycle times  $\omega_k^i, \omega_i$ , startup times  $t_k^i, t_i^{\rm in}$ , and average material flow rates  $D_k^j, D_i$ . The startup time  $t_i^{\rm out}$  is converted into  $t_i^{\rm in}$  by Eq. 1. Equation 7 can be transformed into the following expression in terms of the independent variables by using Eqs. 4 and 6

$$TC = \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \left[ \frac{A_k^{(j)}}{\omega_k^j} \right] + \sum_{i=1}^{|I|} \left[ \frac{A_i}{\omega_i} \right] + \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \left[ P_k^j D_k^j \right]$$

$$+ \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \left[ \left( \frac{H^j}{2} + b^j \right) (1 - x_k^j) + a_k^j \right] D_k^j \omega_k^j$$

$$- \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} (H^j + b^j) D_k^j t_k^j$$

$$+ \sum_{i=1}^{|I|} a_i D_i \omega_i + \sum_{j=1}^{|J|} \sum_{i=1}^{|I|} (H^j + b^j) (f_i^j - g_i^j) D_i t_i^{\text{in}}$$

$$- \sum_{j=1}^{|J|} \sum_{i=1}^{|I|} \frac{H^j}{2} \left[ (1 - x_i^{\text{in}}) f_i^j + (1 - x_i^{\text{out}}) g_{(i)}^j \right] D_i \omega_i + \text{constants}$$

$$(8)$$

where constants are

constants = 
$$\sum_{j=1}^{|J|} (H^{j} + b^{j}) V^{j}(0)$$

$$- \sum_{j=1}^{|J|} \sum_{m=1}^{|M(j)|} \left(\frac{H^{j}}{2}\right) (1 - x_{m}^{j}) D_{m}^{j} \omega_{m}^{j}$$

$$+ \sum_{j=1}^{|J|} \sum_{m=1}^{|M(j)|} (H^{j} + b^{j}) D_{m}^{j} t_{m}^{j} \quad (9)$$

The inventory holdup  $V^j(t)$  should be confined within the storage capacity. Sufficient conditions are  $0 \le \underline{V}^j < \overline{V}^j \le V_{\max}^j$ . Since the storage size  $V_{\max}^j$  should be determined through this analysis, only the conditions  $0 \le V^j$  are necessary. The lower bounds of holdup Eq. 5 are given by the following inequality

$$V^{j}(0) - \sum_{k=1}^{|K(j)|} D_{k}^{j} t_{k}^{j} - \sum_{i=1}^{|I|} g_{i}^{j} D_{i} t_{i}^{\text{out}} - \sum_{i=1}^{|I|} \left(1 - x_{i}^{\text{in}}\right) f_{i}^{j} D_{i} \omega_{i}$$

$$+ \sum_{i=1}^{|I|} f_{i}^{j} D_{i} t_{i}^{\text{in}} - \sum_{m=1}^{|M(j)|} \left(1 - x_{m}^{j}\right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \ge 0 \quad (10)$$

The problem is defined as minimizing the total cost given by Eq. 8 subject to the constraints Eq. 10 with respect to the non-negative design variables  $\omega_k^j$ ,  $\omega_i$ ,  $t_k^j$ ,  $t_i^{\text{in}}$ , and  $D_k^j$ ,  $D_i$ . (We can easily incorporate the upper and/or lower bounded case of design variables, as will be discussed in Example Plant Design and Discussions.) The objective function Eq. 8 is convex and the constraints are linear with respect to  $\omega_k^j, \omega_i$ , and  $t_k^j, t_i^{\text{in}}$ if  $D_k^j, D_i$  are considered as parameters. However, the convexity with respect to  $D_k^j, D_i$  is not clear. At first, we obtain the solution for Kuhn-Tucker conditions with respect to  $\omega_k^j, \omega_i$ and  $t_k^i, t_i^{\text{in}}$  when  $D_k^i, D_i$  are considered as parameters and, then, we will further solve the problem with respect to  $D_k^j, D_i$ . Even though the problem is separated into a two-level parametric optimization problem, the Kuhn-Tucker conditions of the original problem and the two-level problem are the same if the constraints are reduced to equality (Appendix A). The first problem of the two-level problem has a convex objective with linear inequality constraints, and the second problem of the two-level problem has a concave objective with linear equality constraints. The two-level parametric approach leads to global optimum as far as the second problem converges to its global optimum point.

# **Solution of Kuhn-Tucker Conditions**

The Kuhn-Tucker solution to the first level optimization problem minimizing the objective function (Eq. 8) subject to the constraint (Eq. 10) with fixed values of  $D_k^i, D_i$  is obtained by similar algebraic manipulation in Yi and Reklaitis (2002), as is summarized in Appendix B. Optimal cycle times are

$$\omega_k^j = \sqrt{\frac{A_k^j}{D_k^j \Psi_k^j}} \tag{11}$$

$$\omega_i = \sqrt{\frac{A_i}{D_i \Psi_i}} \tag{12}$$

where

$$\Psi_k^j = \left(\frac{H^j}{2} + b^j\right) (1 - x_k^j) + a_k^j \tag{13}$$

$$\Psi_i = a_i + (1 - x_i^{\text{in}}) \sum_{j=1}^{|J|} \left(\frac{H^j}{2} + b^j\right) f_i^j$$

$$+(1-x_i^{\text{out}})\sum_{j=1}^{|J|} \left(\frac{H^j}{2}+b^j\right) g_i^j$$
 (14)

Optimal startup times are

$$\sum_{k=1}^{|K(j)|} D_k^j t_k^j + \sum_{i=1}^{|I|} \left( g_i^j - f_i^j \right) D_i t_i^{\text{in}}$$

$$= V^j(0) - \sum_{m=1}^{|M(j)|} \left( 1 - x_m^j \right) D_m^j \omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j$$

$$- \sum_{i=1}^{|I|} \left[ \left( 1 - x_i^{\text{in}} \right) f_i^j + \left( 1 - x_i^{\text{out}} \right) g_i^j \right] D_i \omega_i$$
(15)

Equation 15 has |K(j)|+|I| variables and |J| equations. In most real cases, the variables outnumber the equations. We may need a secondary objective function to fix the additional freedom and it will be introduced in an example design problem. Optimal storage sizes are

$$V_{s}^{j} = \sum_{i=1}^{|I|} \left[ \left( 1 - x_{i}^{\text{in}} \right) f_{i}^{j} + \left( 1 - x_{i}^{\text{out}} \right) g_{i}^{j} \right] D_{i} \omega_{i}$$

$$+ \sum_{k=1}^{|K(j)|} \left( 1 - x_{k}^{j} \right) D_{k}^{j} \omega_{k}^{j} + \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} \quad (16)$$

Optimal objective value is

$$TC(D_{k}^{j}, D_{i}) = 2 \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \sqrt{A_{k}^{j} \Psi_{k}^{j} D_{k}^{j}} + \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} \left[ P_{k}^{j} D_{k}^{j} \right]$$

$$+ 2 \sum_{i=1}^{|I|} \sqrt{A_{i} \Psi_{i} D_{i}} + \sum_{j=1}^{|J|} \left( \frac{H^{j}}{2} + b^{j} \right) \sum_{m=1}^{|M(j)|} D_{m}^{j} \omega_{m}^{j} (1 - x_{m}^{j})$$

$$(17)$$

The second level optimization is composed of minimizing the objective function Eq. 17 subject to the constraint Eq. 2 with respect to average flow rates  $D_k^j, D_i$ . This optimization problem is in the category of separable concave objective minimization network flow problem. An efficient, but complicated, nonlinear branch-and-reduce algorithm has been published in Shectman and Sahinidis (1998). A rather simple mixed integer linear model that piecewisely linearize the concave objective function has been suggested in Tsiakis et al. (2001). As far as the average flow rates are determined, the other design variables are explicitly calculated by Eqs. 11–16. We will introduce a special case that the average material flow rates are analytically determined.

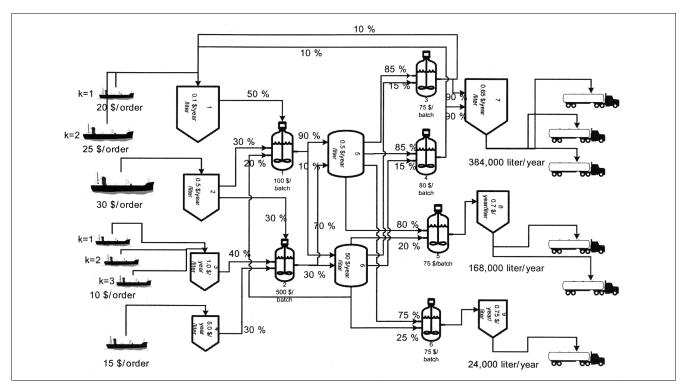


Figure 5. Example plant-input data.

Process groups with the same feedstock composition and product yield commonly occur in chemical plants. The same processes can be built one after the other in order to meet slowly increasing customer demand. Some processes should be built in multiple units, because they reach the capacity limits that originate from technical and/or safety concern. In this article, the process is characterized by the parameters of feedstock composition, product yield, storage operation time fraction, setup cost, and capital cost. It is certain that the identical processes, which have all the same parameters, can be considered as one process. The processes that have the same feedstock composition and product yield, but have different storage operation time fraction, setup cost, and capital cost are called similar processes. The batch process set  $I = \{i\}$ can be regrouped into a similar process set  $L = \{l\}$ , where the process  $i \in l$  has the same feedstock composition and product yield, that is,  $g_{i_1}^j - f_{i_1}^j = g_{i_2}^j - f_{i_2}^j$ , for  $i_1, i_2 \in l$ . Without loss of generality, the second level optimization problem can be decomposed into three optimization problems

Main Problem:

$$\min_{D_{pur}^{j}, D_{l}} \sum_{j=1}^{|J|} \sqrt{A_{k^{*}}^{j} \Psi_{k^{*}}^{j} D_{pur}^{j}} + \sum_{j=1}^{|J|} P_{k^{*}}^{j} D_{pur}^{j} + \sum_{l=1}^{|L|} \sqrt{A_{l} \Psi_{l} D_{l}}$$
(18)

Subject to 
$$D_{pur}^{j} + \sum_{l=1}^{|L|} (g_{l}^{j} - f_{l}^{j}) D_{l} = \sum_{m=1}^{|M(j)|} D_{m}^{j}$$
 (19)

Supplier Selection Problem:

$$\min_{D_k^j} \sum_{k=1}^{|K(j)|} \sqrt{A_k^j \Psi_k^j D_k^j} + \sum_{k=1}^{|K(j)|} \left[ P_k^j D_k^j \right]$$
 (20)

Subject to 
$$\sum_{k=1}^{|K(j)|} D_k^j = D_{pur}^j$$
 (21)

Process Selection Problem: 
$$\min_{D_i} \sum_{i=l}^{|I|} \sqrt{A_i \Psi_i D_i}$$
 (22)

Subject to 
$$\sum_{i=l}^{|I|} D_i = D_l$$
 (23)

The objective functions of supplier and process selection problems are minimizing concave functions. The optimum point exists at the edge of feasible zone. Therefore, only one of average flow rates is equal to the right side value of the constraints and all the others are zeros, that is,  $D_{k^*}^j = D_{\text{pur}}^j$ ,  $D_{l^*} = D_l$  and  $D_{k \neq k^*}^j = 0$ ,  $D_{i \neq l^*} = 0$ . If  $D_{\text{pur}}^j$  in Eq. 21 is constant, the optimal solution for the supplier selection problem simply chooses the one  $k^*$  with minimum objective value. If  $D_1$  in Eq. 23 is constant, the optimal solution for the process selection problem simply chooses the one that has the minimum coefficient of  $\hat{A_i\Psi_i}$ , as proved in Proposition II of Yi and Reklaitis (2002). However, the analytical solution for the Main Problem is available only when Eq. 19 can be solved directly. Suppose that the storage set connected with raw material procurement, denoted as  $R \equiv \{r\}$ , is proper subset of total storage set, that is,  $R \subseteq J$ . Also, suppose that the number of storage units that are not in set R is equal to the number of similar processes, that is,  $|J \setminus R| = |L|$ . Then, Eq.

19 is linear and can be transformed into a linear system with the following matrix and vectors

$$\mathbf{R}_{ex} = \begin{bmatrix} 1 & 0 & \dots & 0 & 0 & g_1^1 - f_1^1 & g_2^1 - f_2^1 & \dots & g_{|L|-1}^1 - f_{|L|-1}^1 & g_{|L|}^1 - f_{|L|}^1 \\ 0 & 1 & \dots & 0 & 0 & g_1^2 - f_1^2 & g_2^2 - f_2^2 & \dots & g_{|L|-1}^2 - f_{|L|-1}^2 & g_{|L|}^2 - f_{|L|}^2 \\ \dots & \dots \\ 0 & 0 & \dots & 1 & 0 & g_1^{|R|-1} - f_1^{|R|-1} & g_2^{|R|-1} - f_2^{|R|-1} & \dots & g_{|L|-1}^{|R|-1} - f_{|L|-1}^{|R|-1} & g_{|L|}^{|R|-1} - f_{|L|}^{|R|-1} \\ 0 & 0 & \dots & 0 & 1 & g_1^{|R|} - f_1^{|R|} & g_2^{|R|} - f_2^{|R|} & \dots & g_{|L|-1}^{|R|+1} - f_{|L|-1}^{|R|+1} & g_{|L|}^{|R|-1} - f_{|L|}^{|R|+1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|R|+1} - f_1^{|R|+1} & g_2^{|R|+1} - f_2^{|R|+1} & \dots & g_{|L|-1}^{|R|+1} - f_{|L|-1}^{|R|+1} & g_1^{|R|+1} - f_{|L|}^{|R|+1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|R|+2} - f_1^{|R|+2} & g_2^{|R|+2} - f_2^{|R|+2} & \dots & g_{|L|-1}^{|R|+2} - f_{|L|-1}^{|R|+2} & g_1^{|R|+2} - f_{|L|}^{|R|+2} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|-1} - f_1^{|J|-1} & g_2^{|J|-1} - f_2^{|J|-1} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|} - f_1^{|J|} & g_2^{|J|-1} - f_2^{|J|} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|} - f_1^{|J|} & g_2^{|J|-1} - f_2^{|J|} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|} - f_1^{|J|} & g_2^{|J|-1} - f_2^{|J|} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|-1} - f_1^{|J|-1} & g_2^{|J|-1} - f_2^{|J|-1} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|-1} - f_1^{|J|-1} & g_2^{|J|-1} - f_2^{|J|-1} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|-1} - f_1^{|J|-1} & g_2^{|J|-1} - f_2^{|J|-1} & \dots & g_{|L|-1}^{|J|-1} - f_{|L|-1}^{|J|-1} & g_1^{|J|-1} - f_1^{|J|-1} \\ 0 & 0 & \dots & 0 & 0 & g_1^{|J|-1} - f_1^{|J|-1} & g_2^{|J|-1} - f_2^{|J|-1} & \dots & g_1^{|J|-1} - f_1^{|J|-1} & g_2^{|J|-1} - f$$

$$\boldsymbol{D_{RL}} = \left\{ D_{pur}^{1}, \ D_{pur}^{2}, \ \dots, \ D_{pur}^{|R|}, \ D_{1}, \ D_{2}, \ \dots, \ D_{|L|-1}, \ D_{|L|} \right\}^{T}, \qquad \boldsymbol{D_{out}} = \left\{ \sum_{m=1}^{|M(j)|} D_{m}^{j} \right\}^{T}$$

$$(24)$$

The solution for Eq. 19 exists if  $\det(R_{ex}) \neq 0$  and  $(R_{ex})^T D_{\text{out}} > 0$ . The second condition is necessary to guarantee the non-negative element values of  $D_{RL}$  from Fakas's theorem in Prekopa (1995)

$$D_{RL} = (R_{ex})^{-1} D_{out} \tag{25}$$

Note that the optimal average material flow rates for the sequential multistage case derived in Yi and Reklaitis (2002) coincide with Eq. 25.

Design computation proceeds in the reverse of the mathematical derivation so far. First of all, the average flow rates should be computed by Eq. 25 and/or Eqs. 18–23. Then, cycle times are calculated by Eqs. 11 and 12. Finally, startup times and storage sizes are calculated by Eqs. 15 and 16. Equation 15 is a linear system and also can be represented by a matrix-vector equation. Define vector  $T_{RL}$  and  $\Lambda$  (0) as follows

$$T_{RL} = \left\{ t_k^{1}, t_k^{2}, \dots, t_k^{|R|}, t_1^{\text{in}}, t_2^{\text{in}}, \dots, t_{|L|-1}^{\text{in}}, t_{|L|}^{\text{in}} \right\}^T$$

$$\Lambda(\mathbf{0}) = \left\{ V^j(0) - \sum_{m=1}^{|M(j)|} (1 - x_m^j) D_m^j \omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j - \sum_{i=1}^{|I|} \left[ (1 - x_i^{\text{in}}) f_i^j + (1 - x_i^{\text{out}}) g_i^j \right] D_i \omega_i \right\}^T$$
(26)

The corresponding matrix-vector equation for Eq. 15 is

$$(R_{ex})(I_{ex}D_{RL})T_{RL} = \Lambda(0) \tag{27}$$

where  $I_{ex}$  is a unit matrix that has the same dimension with  $R_{ex}$ . In order for Eq. 27 to have the non-negative elements of solution vector  $T_{RL}$ , the condition  $[(R_{ex})(I_{ex}D_{RL})]^T\Lambda(\mathbf{0}) > \mathbf{0}$  should be satisfied.

## **Example Plant Design and Discussions**

The example plant in Figure 5 has a similar structure and parametric values to the example in Yi and Reklaitis (2002), except that this example has recycle streams. The output products of downstream processes 3 and 4 are fed into upstream storage 1. The product in storage 6 is recycled into process 1. The input data as well as computed results are summarized in Tables 1–4. Then,  $R_{ex}$  is

We can easily find that  $R_{ex}$  is invertible and the average flow rates in  $D_{RL}$  can be calculated by Eq. 25. We assume that the purchasing average material flow rate from each supplier has the lower bound of 10,000 L/year and the average material flow rates through processes 3 and 4 have the lower bound of 100,000 L/year. Then, optimal average flow rates from suppliers for the same raw material are determined so that the supplier with minimum  $A_k^j \Psi_k^j$  has maximum possible flow rate and the other suppliers have their minimum flow rates. The flow rates for similar processes 3 and 4 are determined by the same reasoning. After calculating the average material flow rates, Eqs. 11 and 12 give optimal batch sizes directly. The deadline of first finished product delivery to customer is set to 0.3 years later. The startup times of processes are subsequently calculated by Eq. 15. The variables in Eq. 15 outnumber the equations. The additional freedom can be used for convenient and economic startup sequence. We would like

Table 1. Input and Output Data with Respect to Process

Process	$D_i$	$B_i$	$\omega_i$	$t_i^{\mathrm{in}}$	$t_i^{\text{out}}$	$x_i^{\text{in}}, x_i^{\text{out}}$	$a_i$	$A_i$
I1	241,176	113	0.0005	0.2981	0.2985	0	1,825	100
I2	425,725	336	0.0008	0.2969	0.2977	0	1,825	500
I3	326,667	239	0.0007	0.2989	0.2996	0	365	75
<b>I</b> 4	100,000	136	0.0014	0.3000	0.3014	0	365	80
I5	168,000	171	0.0010	0.2990	0.3000	0	365	75
I6	24,000	64	0.0027	0.2973	0.3000	0	365	75

Table 2. Input and Output Data with Respect to Feedstock Storage and Supplier

Storage	Supplier	$D_k^j$	$B_k^j$	$\boldsymbol{\omega}_k^j$	$t_k^j$	$x_k^j, a_k^j$	$A_k^j$
J1	K1	67,922	272	0.0040	0.2954	0	20
J1	K2	10,000	117	0.0117	0.3000	0	25
J2	<b>K</b> 1	200,071	570	0.0028	0.2965	0	30
J3	<b>K</b> 1	150,290	283	0.0019	0.2954	0	10
J3	K2	10,000	73	0.0073	0.3000	0	10
J3	K3	10,000	73	0.0073	0.3000	0	10
J4	K1	127,718	304	0.0024	0.2959	0	15

Table 3. Input Output Data with Respect to Storage

Storage	$V^{j}(0)$	$V_s^j$	$H^{j}$	$b^j$	$\sum_{m=1}^{ M(j) } D_m^j$
J1	0	483	0.1	18.25	0
J2	0	704	0.5	18.25	0
J3	0	563	1	18.25	0
J4	0	405	5	18.25	0
J5	0	840	0.5	36.5	0
J6	0	241	50	36.5	0
J7	0	337	0.65	25.55	384,000
J8	0	171	0.7	25.55	168,000
<b>J</b> 9	0	64	0.75	25.55	24,000

to minimize the initial inventory of intermediate materials, because they should be purchased from other companies, probably competitors. Also, we would like to postpone the startup times as much as possible to be just in time to the first delivery time of 0.3 years. We can formulate a subsidiary optimization problem to minimize

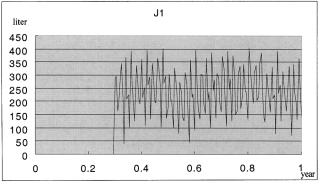
$$10^4 \sum_{j=1}^{|J|} V^j(0) - \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} t_k^j - \sum_{i=1}^{|I|} t_i^{\text{in}}$$

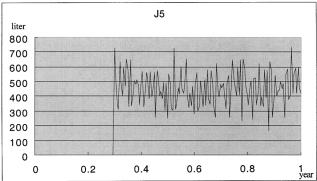
subject to Eq. 15. Calculated results are summarized in Tables 1-4. Figure 6 shows the inventory profiles of selected storages predicted from Eq. 3 based on optimal design calculation results. The resulting sizes of batch processes and storage units are quite small, because we have considered capital costs of those equipments when  $\Psi_k^j$  and  $\Psi_i$  were calculated by Eqs. 13 and 14. According to our theory, the optimality cannot be realized by manipulating only design variables such as equipment sizes, but can be achieved by manipulating both design and operating variables such as startup times and initial inventory levels. The output data in Tables 1–3 show such results. In spite of complicated recycle streams, proper process startup sequence, as well as optimal equipment sizes, is easily found. Note that one of the feedstock materials to process 1 is the product of process 2. Therefore, process 2 should start up earlier than process 1 in order for the material in storage 6 to be available to feed to process 1, as can be seen at Table 1.

We would like to discuss the inclusion of more constraints into the model. The design variables are mostly upper and lower bounded in real applications. We already have dealt with the lower bound of average flow rates in the above example where the minimum average flow rates were 10,000 and 100,000 for suppliers and processes 3 and 4, respectively. If cycle times and/or startup times are out of upper and/or lower bounds, either upper or lower bound close to the unbounded optimal solution should be selected because the ob-

Table 4. Feedstock Composition and Product Yield

Process	Storage	$f_i^j$	$g_i^j$	Process	Storage	$f_i^j$	$g_i^j$
11	J1	0.50	0.00	I3	J6	0.15	0.00
I1	J2	0.30	0.00	I3	J7	0.00	0.90
I1	J5	0.00	0.90	<b>I</b> 4	J1	0.00	0.10
I1	J6	0.20	0.10	<b>I</b> 4	J5	0.85	0.00
I2	J2	0.30	0.00	<b>I</b> 4	J6	0.15	0.00
I2	J3	0.40	0.00	<b>I</b> 4	J7	0.00	0.90
I2	J4	0.30	0.00	I5	J5	0.80	0.00
I2	J5	0.00	0.70	I5	J6	0.20	0.00
12	J6	0.00	0.30	I5	Ј8	0.00	1.00
I3	J1	0.00	0.10	<b>I</b> 6	J5	0.75	0.00
I3 J5	J5	0.85	0.00	<b>I</b> 6	J6	0.25	0.00
				16	<b>J</b> 9	0.00	1.00





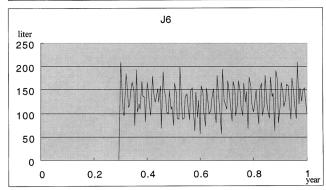


Figure 6. Inventory profiles resulted from optimal design.

jective function is convex with respect to cycle times and startup times in the first optimization problem.

## Conclusion

3092

This study deals with the optimal design of a chemical plant composed of a set of storage units and a set of batch processes in most general network structure. The material in a storage unit can be purchased, internally produced, internally consumed, and/or sold out. A process can consume multiple materials in storage units and produce multiple products into storage units. All operations are assumed to be periodical. Startup time and cycle time of any process are our major decision variables with average material flow rate through the process. The economic factors considered in this study cover raw material purchase cost, setup cost, inventory holding cost, and capital cost of construction. Sequence dependent setup cost and backlogging cost are not considered in this study. Analytical optimal solution for the design problem indicates that the design procedure can be decomposed into two phases: (1) To determine the average material flow rates by solving a separable concave minimization network flow problem; (2) To determine the cycle times and startup times by simple analytical equations. Solving concave minimization problem is nontrivial work, but an analytical solution is available in a special case. The average material flow rates can be calculated by any other method, such as linear programming, without damaging the optimality of the other procedure.

Because the network model is very general, the result can be applicable to the plant involving recycling streams which is known as very difficult to solve, but also very popular in chemical industries. In spite of enlarged applicability, the derivation and results in this study are much more compact than our previous work in Yi and Reklaitis (2002). Although this study is focused on plant design problem, the application is not limited to the design. Simple analytical optimal solution of cycle times and startup times can contribute to the optimal operation of the plant. The supplier selection problem of Eqs. 20 and 21 may be very useful especially to choose the best suppliers of raw materials, as it is obviously one of most important operational issues in manufacturing business.

# **Acknowledgment**

This work was supported by a Grant No.(R01-2002-000-00007-0) from Korea Science & Engineering Foundation.

## **Notation**

```
a_k^i = annualized capital cost of raw material purchasing facility,
     dollars per unit of item per year
```

 $a_i$  = annualized capital cost of unit i, dollars per unit of item per year

 $b^{j}$  = annualized capital cost of storage facility, dollars per unit of item per year

 $A_k^i$  = ordering cost of feedstock materials, dollar per order

 $A_i =$  ordering cost of noncontinuous units, dollar per order

 $B_k^{j}$  = raw material order size, units per lot

 $\vec{B}_i$  = noncontinuous unit size, units per lot

 $B_m^j$  = final product delivery size, units per lot

 $D_k^j$  = average material flow of raw material supply, units per year

 $D_{m}^{j}$  = average material flow of customer demand, units per year

 $\vec{D}_i$  = average material flow through noncontinuous units, units per vear

 $D_{RL}$  = defined by Eq. 24

 $D_{\text{out}} = \text{defined by Eq. 24}$ 

= feedstock composition of unit i

= product yield of unit i

 $H^{ij}$  = annual inventory holding costs, dollars per unit of item per vear

I = noncontinuous process set

 $I_{ex} = \text{unit matrix}$ 

 $\hat{J} = \text{storage set}$ 

K(j) = raw material supplier set for storage j

M(j) = consumer set for storage j

 $P_k^j$  = price of raw material j from supplier k

R = subset of storage connected with raw material suppliers

 $R_{ex}$  = defined by Eq. 24

= startup time of customer demand

 $t_i^j$  = startup time of customer demand  $t_i^m$  = startup time of feedstock feeding to noncontinuous unit i $t_i^{\text{out}} = \text{startup}$  time of product discharging from noncontinuous

December 2003 Vol. 49, No. 12 **AIChE Journal** 

unit i

 $t_R^{j}$  = startup time of raw material purchasing  $T_{RL}$  = defined by Eq. 26  $\overline{V}^{j}$  = upper bound of inventory holdup, units of item

 $V^{j}$  = lower bound of inventory holdup, units of item

 $V^{j}(t)$  = inventory holdup, units of item

 $V^{j}(0)$  = initial inventory holdup, units of item

 $V_{\text{max}}^{j}$  = storage size, units of item

 $x_k^j$  = storage operation time fraction of purchasing raw materials  $x_i^{in}$  = storage operation time fraction of  $x_i^{in}$ unit i

 $x_i^{\text{out}}$  = storage operation time fraction of discharging from noncontinuous unit i

 $x_m^j$  = storage operation time fraction of customer demand

#### Greek letters

 $\omega_m^j$  = cycle time of customer demand, year

 $\omega_k^j$  = cycle time of raw material purchasing, year

 $\omega_i$  = cycle time of noncontinuous units, year

 $\Lambda(\mathbf{0}) = \text{defined by Eq. 26}$ 

 $\Psi_i$  = defined by Eq. 13  $\Psi_k^j$  = defined by Eq. 14

### **Subscripts**

i = noncontinuous unit index

l = similar process group index

k = raw material vendors

m = finished product customers

## Superscripts

i = storage index

r = storage index connected with raw material suppliers

#### Special functions

int[·] = truncation function to make integer

 $res[\cdot] = positive residual function to be truncated$ 

|X| = number of elements in set X

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## Appendix A

Proof of statement that Kuhn-Tucker condition of two-level parametric optimization problem are the same as those of the original optimization problem if the constraints become equalities.

We will consider only one variable, one parameter, and one

constraint, however, the development can be readily expanded to the case with multiple variables, parameters, and constraints without loss of generality. Consider the following optimization problem

$$\min_{x,y} f(x,y) \text{ subject to } g(x,y) \ge 0$$
 (A1)

The Kuhn-Tucker conditions for Eq. A1 are

$$\frac{\partial f(x,y)}{\partial x} - \lambda \frac{\partial g(x,y)}{\partial x} = 0$$

$$\frac{\partial f(x,y)}{\partial y} - \lambda \frac{\partial g(x,y)}{\partial y} = 0$$

$$\lambda g(x,y) = 0$$

$$\lambda \ge 0$$
(A2)

Now, consider the optimization problem Eq. A1 separated into a two-level parametric problem. At first, suppose y to be a fixed parameter. The first level optimization problem is

$$\min_{x} f(x,y)$$
 subject to  $g(x,y) \ge 0$ ,  $\forall y$  (A3)

The Kuhn-Tucker conditions for Eq. A3 are

$$\frac{\partial f(x,y)}{\partial x} - \lambda \frac{\partial g(x,y)}{\partial x} = 0$$

$$\lambda g(x,y) = 0$$

$$\lambda \ge 0 \tag{A4}$$

Let  $\bar{x}(y)$  and  $\bar{\lambda}(y)$  be the solution of Eq. A4. Suppose that  $g(\bar{x}(y),y) = 0$ . Then, the second level optimization is

$$\min_{y} f(\bar{x}(y), y) \text{ subject to } g(\bar{x}(y), y) = 0$$
 (A5)

The Kuhn-Tucker condition is

$$\frac{df(\bar{x}(y),y)}{dy} - \lambda' \frac{dg(\bar{x}(y),y)}{dy} = 0$$
 (A6)

3093

Note that, although Eq. A6 includes total differentiation, it can be reduced to partial differentiation if the chain rule is applied to Eq. A6 with  $\lambda' = \overline{\lambda}(y)$ 

$$\frac{df}{dy} - \lambda' \frac{dg}{dy} = \frac{\partial f}{\partial x} \frac{\partial x}{\partial y} + \frac{\partial f}{\partial y} - \lambda' \left[ \frac{\partial g}{\partial x} \frac{\partial x}{\partial y} + \frac{\partial g}{\partial y} \right]$$

$$= \left[ \frac{\partial f}{\partial x} - \lambda' \frac{\partial g}{\partial x} \right] \frac{\partial x}{\partial y} + \frac{\partial f}{\partial y} - \lambda' \frac{\partial g}{\partial y}$$

$$= \frac{\partial f}{\partial y} - \lambda' \frac{\partial g}{\partial y} = 0 \quad (A7)$$

Equations A4 and A7 coincide with Eq. A2 under the assumption of  $g(\bar{x}(y),y) = 0$ . This proves our statements.

## Appendix B

Kuhn-Tucker solution to the first level optimization problem.

The Lagrangian for the optimization problem to minimize Eq. 8 subject to Eq. 10 with respect to  $\omega_k^i$ ,  $\omega_i$ ,  $t_k^j$ ,  $t_i^{\text{in}}$  is

$$L = TC$$

$$-\sum_{j=1}^{|J|} \lambda^{j} \left[ V^{j}(0) - \sum_{k=1}^{|K(j)|} D_{k}^{j} t_{k}^{(j)} - \sum_{i=1}^{|I|} g_{i}^{j} D_{i} \left[ t_{k}^{\text{in}} + \omega_{i} \left( 1 - x_{i}^{\text{out}} \right) \right] \right]$$

$$-\sum_{i=1}^{|I|} \left( 1 - x_{i}^{\text{in}} \right) f_{i}^{j} D_{i} \omega_{i}$$

$$-\sum_{i=1}^{|I|} \left( 1 - x_{i}^{\text{in}} \right) f_{i}^{j} D_{i} \omega_{i} + \sum_{i=1}^{|I|} f_{i}^{j} D_{i} t_{i}^{\text{in}} - \sum_{i=1}^{|I|} \left( 1 - x_{i}^{\text{in}} \right) f_{i}^{j} D_{i}^{j} \omega_{i} + \sum_{m=1}^{|I|} f_{m}^{j} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|I|} f_{i}^{j} D_{i} t_{i}^{\text{in}} - \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right]$$

$$+ \sum_{i=1}^{|M(j)|} \left[ \sum_{m=1}^{|M(j)|} \left( 1 - x_{m}^{j} \right) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} \omega_{m}^{j} \right]$$

where  $\lambda^{j}$  is the Lagrange multiplier. Kuhn-Tucker conditions give

$$\frac{\partial L}{\partial t_k^j} = -\left(H^j + b^j\right)D_k^j + \lambda_{lb}^j D_k^j = 0$$
 (B2)

$$\frac{\partial L}{\partial \omega_k^j} = -\frac{A_k^j}{\left(\omega_k^j\right)^2} + \left[ \left(\frac{H^j}{2} + b^j\right) \left(1 - x_k^j\right) + a_k^j \right] D_k^j = 0 \quad (B3)$$

$$\frac{\partial L}{\partial t_i^{\text{in}}} = \sum_{j=1}^{|J|} (H^j + b^j) (f_i^j - g_i^j) D_i - \sum_{j=1}^{|J|} \lambda_{lb}^j (f_i^j - g_i^j) D_i = 0$$

$$\frac{\partial L}{\partial \omega_i} = -\frac{A_i}{\left(\omega_i\right)^2} + a_i D_i - \sum_{j=1}^{|J|} \frac{H^j}{2} \left[ \left(1 - x_i^{\text{in}}\right) f_i^j \right]$$

$$+\left(1-x_i^{\text{out}}\right)g_i^j\right]D_i$$

$$+ \sum_{j=1}^{|J|} \lambda^{j} \left[ \left( 1 - x_{i}^{\text{in}} \right) f_{i}^{j} + \left( 1 - x_{i}^{\text{out}} \right) g_{i}^{j} \right] D_{i} = 0 \quad \text{(B5)}$$

$$\lambda^{j} \left[ V^{j}(0) - \sum_{k=1}^{|K(j)|} D_{k}^{j} t_{k}^{j} - \sum_{i=1}^{|I|} g_{i}^{j} D_{i} \left[ t_{i}^{\text{in}} + \omega_{i} (1 - x_{i}^{\text{out}}) \right] - \sum_{i=1}^{|I|} (1 - x_{i}^{\text{in}}) f_{i}^{j} D_{i} \omega_{i} + \sum_{i=1}^{|I|} f_{i}^{j} D_{i} t_{i}^{\text{in}} - \sum_{m=1}^{|M(j)|} (1 - x_{m}^{j}) D_{m}^{j} \omega_{m}^{j} + \sum_{m=1}^{|M(j)|} D_{m}^{j} t_{m}^{j} \right] = 0 \quad (B6)$$

Solving Eqs. B2 and B4 gives

$$\lambda^j = H^j + b^j \tag{B7}$$

Solving Eqs. B3 and B5 with Eq. B7 gives Eqs. 11 and 12 in the main text. Solving Eq. B6 gives Eq. 15 in the main text.

Manuscript received Sept. 23, 2002, and revision received May 24, 2003.

(B4)