

# Optimal Design of Batch-Storage Network Using Periodic Square Wave Model

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*This study is to find the analytic solution for determining the optimal capacity (lot size) of a multiproduct, sequential, multistage production and inventory system to meet the finished product demand. It overcame the limitation of the classical lot sizing method developed based on the single product and single-stage assumption. The superstructure of the plant consisted of a network of serially and/or parallel interlinked batch processes and storage units. The processes involve chemical reactions with multiple feedstock materials and multiple products, as well as mixing, splitting, or transportation of materials. The objective function for optimization is minimizing the total cost composed of setup and inventory holding costs, as well as the capital costs of constructing processes and storage units. The resulting simple analytic solution can greatly enhance the proper and quick investment decision for the preliminary plant design problem confronted with diverse economic situations.*

## Introduction

Intermediate storage constitutes important equipment to mitigate the material flow imbalance of feedstock materials and intermediate products in order to meet finished product demand. Yet, a 1971 study of U. S. refineries showed that 22% of the process unit costs were related to storage. Additionally, inventories represented about 23% of total assets of the average chemical process industries (Kalis, 1986). Increasing storage facilities is no longer a desirable option because of environmental and safety concerns, as well as space shortage and increased land value. Modern storage facilities implement advanced and sophisticated automation systems for the accurate quality control and, therefore, the construction and operating costs of storage facilities are substantial. However, reducing storage capacity can be an extremely painful step in operational practice. A storage capacity shortage can cause many unusual difficulties through the supply and demand chain such as lost sales, feedstock or intermediate product shortage, frequent schedule change, and so on. In principle, there must be an optimal point of storage capacity, although it may be very difficult to find.

At the early stage of plant design, designers would like to determine a quick and rough estimate of process and storage capacities to meet estimated finished product demand. The

classical economic lot size model, the so-called Economic Order Quantity (EOQ) or Economic Production Quantity (EPQ) model, is most appropriate for this purpose. However, the EOQ/EPQ model gives unreliable predictions when it is applied to a multiproduct, multistage system. The designers should segregate the multiple stages into many single stages and aggregate the multiple products into a single product because the EOQ/EPQ model was originally developed on the basis of the single product and single stage assumption.

Analytical models are effective tools for intermediate storage analysis. Karimi and Reklaitis (1983) developed analytical results for the case of limiting storage volume in serial systems composed of arbitrary configurations of batch, semi-continuous, or continuous operations. They extended their results to the multiple input/multiple output intermediate storage structure (Karimi and Reklaitis, 1985a), as well as the parametric variation case (Karimi and Reklaitis, 1985b,c). The main idea of their development was to assume periodic material flows, which enabled the use of powerful Fourier series properties. The same method has been applied for the case of periodic material flow including periodic production failure by Lee and Reklaitis (1988, 1989).

This study deals with the development of a compact analytical solution of the optimal lot sizing problem for a multiproduct, sequential multistage production and inventory sys-

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tem with serially and parallel interlinked storage units and processes. The processes involve chemical reactions with multiple feedstock materials and multiple products, as well as mixing, splitting, or transportation of materials. A systematic approach to this design problem can be found in the chemical engineering literature as given by Modi and Karimi (1989). A very detailed batch processing and intermediate storage model was introduced, and the resulting mixed integer non-linear programming formulation was solved by heuristics and mathematical programming techniques. By contrast, to the very limited publication in the chemical engineering literature, the operations research literature is very extensive since the EOQ model has been developed in the early 20th century. The fundamental ideas are summarized well in Muckstadt and Roundy (1993). The basic assumptions on extending the single stage EOQ style model to the general multistage system are summarized as stationary (periodic operation), nested (synchronized operations among stages), and power-of-two (operation period is a multiple of two times the basic operation period). Under these assumptions, an approximating near optimal solution can be developed which is probably within 2% of optimality gap. However, the solution does not guarantee feasibility. Recently, Teo and Bertsimas (2001) suggested a feasible algorithmic solution within a 2% optimality gap. Among the above assumptions, the nestedness and power-of-two assumptions are of questionable applicability to the chemical processes. The key difference between the results in Muckstadt and Roundy (1993) and the results presented here lies in two facts: (a) We consider the time delay which occurs when materials pass through processes and, therefore, the dispatching timing at each storage site is an important decision variable in this study. (b) The process model used in this study can accommodate the chemical reaction from multiple feedstock materials to multiple product materials, which usually happens in chemical plants. In related research, Karimi (1989, 1992) suggested several feasible and optimal algorithmic solutions to the problem without the nestedness and power-of-two assumptions for a

serial multistage system. He pointed out the importance of an initial dispatching time delay between stages. It is one of the results of this study that the optimality of plant design will be realized not only by selecting optimal equipment capacity, but also by selecting optimal initial dispatching time delay between stages.

Figure 1 summarizes the difference in the process description between the EOQ related models in the operations research literature and the PSW model in this study. The EOQ model only deals with the process with a single feed and a single discharge stream as shown in Figure 1a. We introduce feedstock composition (Bill Of Materials) and product yield parameters to describe the chemical reaction with multiple feedstock materials and multiple products, as shown in Figure 1b.

We address a batch-storage network and exclude the details of the operational or design constraints. Instead, we focus on obtaining a compact set of analytical solutions. This 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.

We use a periodic square wave (PSW) model, which was developed in our earlier work (Yi and Reklaitis, 2000). The PSW model is suitable to describe the material flow of highly interlinked batch-storage systems. The PSW model has been successfully applied to the optimal design of multiproduct single stage production and inventory systems in Yi and Reklaitis (2000). The reported analytical solution reduces to the EOQ/EPQ equation when it is applied to a single product single stage system. The optimal lot size calculated by the PSW model is much smaller than that given by the EOQ/EPQ model. The present study is an extension of the previous work

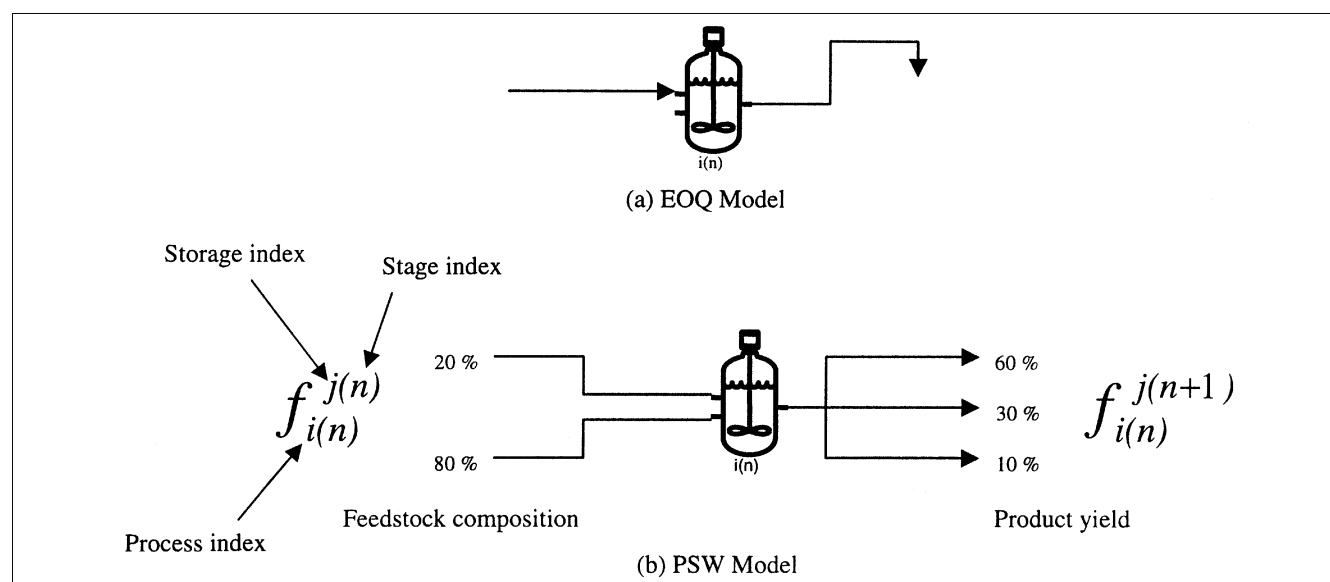


Figure 1. Difference of process representation between EOQ model and PSW model.

of Yi and Reklaitis (2000) to the sequential network structure of batch-storage systems.

### Motivating Plant Design Example

We will introduce a motivating plant design example to emphasize the importance of this study. The plant is composed of two raw materials, two reactors and two products, as shown in Figure 2. Two raw materials and products are stored in their own dedicated storage units. The first product is produced from a 80:20 ratio of the two raw materials, and the second product is produced from a 85:15 ratio of the two raw materials. The inventory holding costs of raw materials and products and the processing setup costs of the two reactors are denoted in Figure 2. We would like to determine the optimal size of the reactors and storage units.

The EOQ method is the current industrial practice for this design problem. When we use the EOQ model, the size of first reactor is

$$\sqrt{\frac{2(\text{Setup Cost})(\text{Average Flow Rate})}{(\text{Product Inventory Holding Cost})}} = \sqrt{\frac{2(75)(38,400)}{(0.65)}} = 2,977 \text{ L}$$

The EOQ model does not consider the effect of raw materials at the above calculation, however, as will be shown the PSW model does. When we use the design equation derived from the PSW model in Yi and Reklaitis (2000), the size of first reactor is

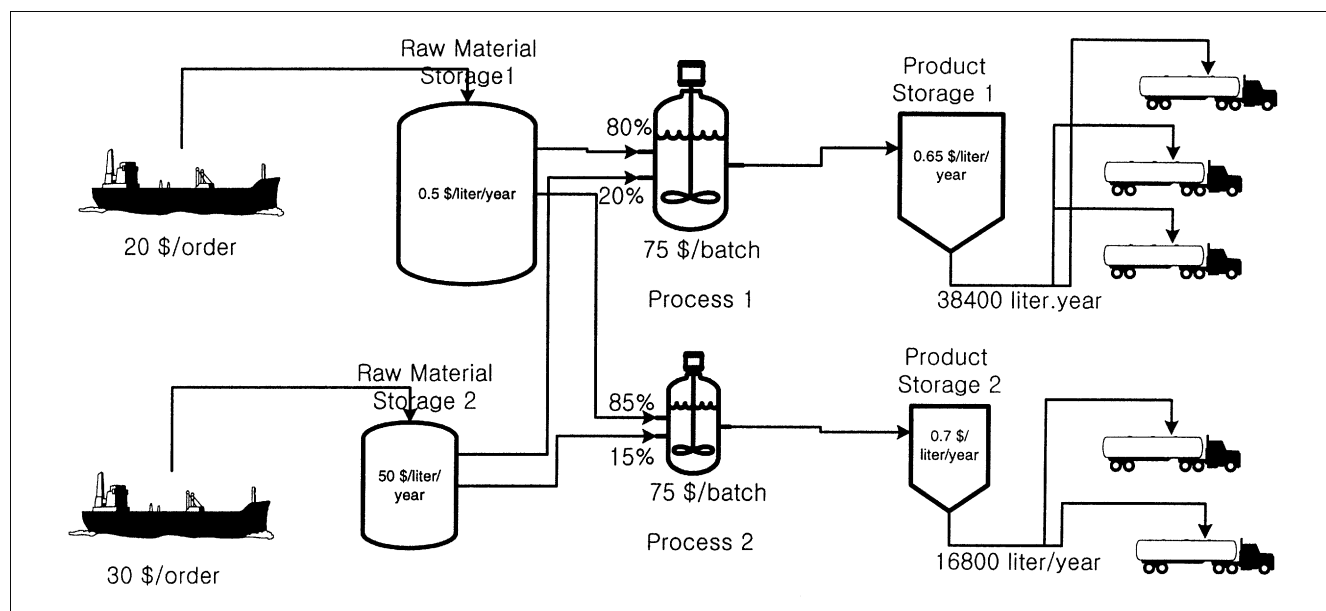
$$\sqrt{\frac{2(\text{Setup Cost})(\text{Average Flow Rate})}{(\sum(\text{Feed Comp})(\text{Feed Inv Hold Cost}) + \sum(\text{Prod Yield})(\text{Prod Inv Hold Cost}))}} = \sqrt{\frac{2(75)(38,400)}{(0.85*0.5 + 0.15*50 + 0.65)}} = 820 \text{ L}$$

**Table 1. Optimal Equipment Sizes Calculated by EOQ and PSW Models**

	EOQ Model	PSW Model
Raw Material	1,957	1,957
1 Order Size		
Raw Material	108	108
2 Order Size		
Raw Material	1,957	3,018
1 Storage		
Raw Material	108	343
2 Storage		
Process 1	2,977	820
Process 2	1,897	476
Product 1	2,977	820
Storage		
Product 2	1,897	476
Storage		

The equipment sizes calculated by the EOQ model and the PSW model are summarized in Table 1. The observation that the reactor sizes calculated by the PSW model are much smaller than those of the EOQ model indicates the possibility that the EOQ solution may not be optimal. Also, the observation that the storage sizes calculated by the PSW model are greater than those of the EOQ model indicates the possibility that the EOQ solution may not be feasible within storage limits. Note that two models gives the same purchase lot size because the EOQ model is a subsystem of the PSW model structure.

The above example is a single-stage problem. For a multi-stage problem, each designer will produce a different solu-



**Figure 2. Motivating example plant design problem.**

tion by using the EOQ model, because the multiple stages can be segregated into many single stages in many different ways in order to meet the EOQ model conditions. Obviously, the EOQ solution for the multistage system will be far from optimality.

The approach taken in this study is not much different from that of EOQ model development in spite of the improved modeling accuracy. In this study, we will prove that the design equations for multiproduct, single-stage system derived in Yi and Reklaitis (2000) are still held as a subsystem of a general multiproduct, multistage system. For the single-stage system in our previous work, average material flow rates through processes and storage units were already known parameters. However, the average flow rates are considered as variables in this multistage system. In the previous work, we confined the network structure to the case in which the number of processes was equal to the number of products, however, in this study, we will enlarge the network structural scope to include the case in which the number of processes is greater than the number of products.

In the following section, we will define the parameters and variables of the batch-storage network structure. We assume that the material flows between processes and storages are periodic square wave shaped. Then, we can calculate the current inventory holdup of each storage unit by using the PSW model. The special properties of the PSW model provide the average and upper/lower bound on the inventory holdup. By using these equations, we can construct a nonlinear optimization model to minimize the total cost consisting of setup costs, inventory holding costs, and equipment capital costs under the constraints of no holdup depletion in all storage units. The design variables are processing cycle times, average material flow rates, and initial delay (dispatching) times. As will be shown, it is possible to find the analytical solution of Kuhn-Tucker conditions of this complicated nonlinear optimization problem. Based on the optimal solution, we will suggest a simple optimal design procedure. The assumptions necessary to obtain the analytical solution are summarized as follows:

- Material flows are periodic square wave shaped.
- Finished product demands are an arbitrary periodic function.
- No stock-outs are allowed in all storage units.
- Feedstock compositions (Bill Of Materials), product yields, and transportation time fractions are constant parameters.
- Processes get all feedstock materials at the same time and discharge products at the same time.
- The number of processes is greater than or equal to the number of products.
- A similar process group consists of the set of processes that have the same product yields. The processes in the same similar group have the same feedstock compositions.

More detailed explanations of these assumptions will be provided in subsequent sections.

## Definition of Parameters and Variables

A chemical plant, which converts raw materials into final products through multiple physicochemical processing steps, is effectively represented by the batch-storage network, as

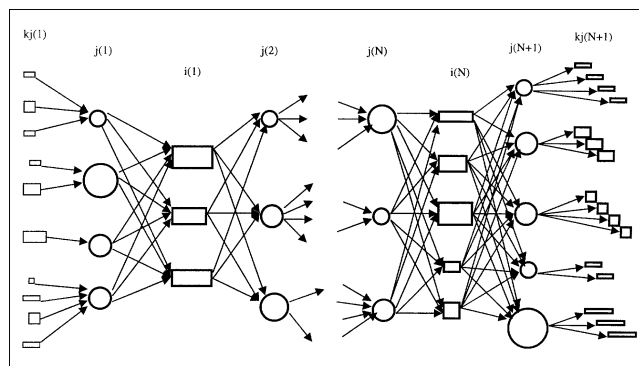


Figure 3. Superstructure of batch-storage network.

shown in Figure 3. The circles in the figure represent storage units, the squares represent batch processes, and the arrows represent the material flows. Each process requires multiple feedstock materials of fixed composition and produces multiple products with a fixed product yields. Each storage unit is dedicated to one material. Multiple storage units that store the same material are considered as one storage unit. The storage index is  $j(n)$  where the stage index  $n$  ( $n = 1, 2, \dots, N + 1$ ) is numbered from left (raw materials) to right (finished products) in Figure 3 and  $j$  ( $j = 1, 2, \dots, |j(n)|$ ) is numbered from the top circle to the bottom circle in Figure 3. Therefore, the raw material storage index is superscript  $j(1)$  and the final product storage index is  $j(N + 1)$ . For example, the size of storage  $j(n)$  is  $V_s^{j(n)}$ . Figure 4 presents a more detailed configuration of the  $n$ -th stage. The material consumption processes of the  $n$ -th stage are denoted by subscript  $i(n)$  ( $i = 1, 2, \dots, |i(n)|$ ) from the top square to the bottom square in Figure 4. For example, the batch size of process  $i(n)$  is denoted by  $B_{i(n)}$ . The processes denoted by subscript  $i(n)$  are confined within the plant boundary. Both raw material pur-

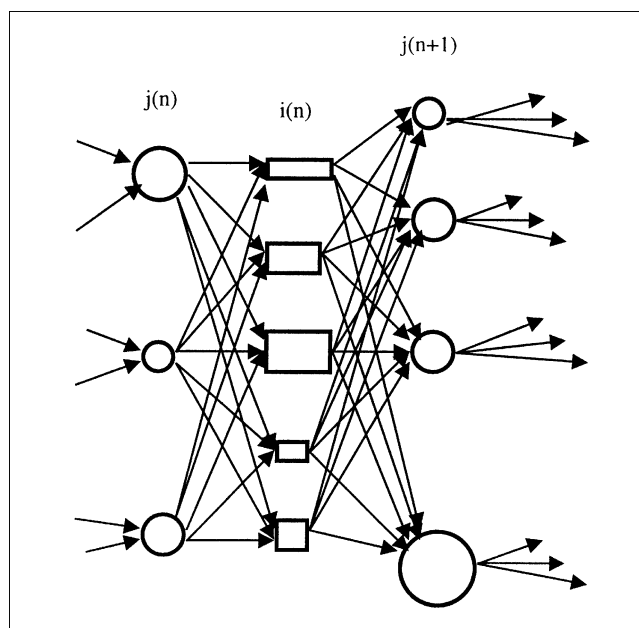


Figure 4. The  $n$ -th stage.

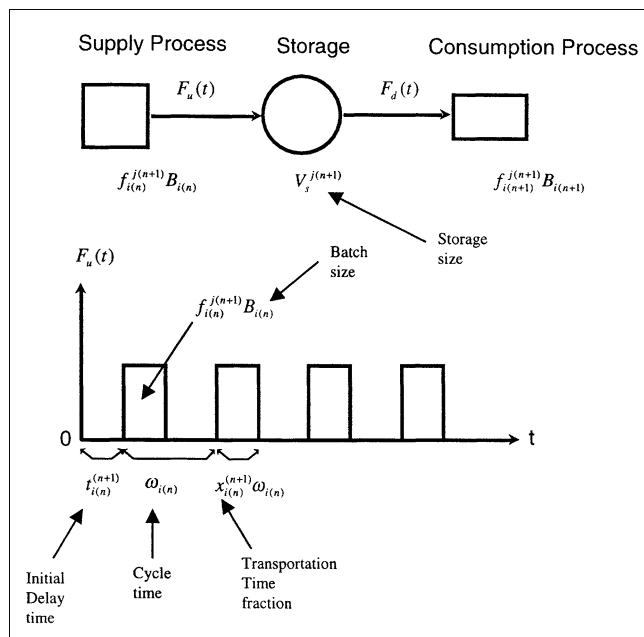


Figure 5. Flow of periodic square wave model.

chase and finished product sales, which connect the plant with the outside world, are denoted by superscript  $j(1)$  and  $j(N+1)$ , respectively, with subscript  $k, m$  where  $k$  denotes the supplier and  $m$  denotes the customer index. For example, the purchasing lot size of raw material  $j(1)$  from supplier  $k$  is denoted by  $B_m^{j(1)}$  and the sales lot size of finished product  $j(N+1)$  to customer  $m$  is denoted by  $B_m^{j(N+1)}$ . The number of consumption processes in the  $n$ -th stage is denoted by  $|i(n)|$  and the number of storage units in  $n$ -th stage is denoted by  $|j(n)|$ . The number of suppliers for raw material  $j(1)$  is denoted by  $|kj(1)|$  and the number of customers for finished product  $j(N+1)$  is denoted by  $|mj(N+1)|$ . The feedstock materials of process  $i(n)$  are the intermediate products stored in storage  $j(n)$ , and the feedstock composition (Bill Of Materials) is denoted by  $f_{i(n)}^{j(n)}$ , as shown in Figure 1b. The product indices of process  $i(n)$  are the intermediate products stored in storage  $j(n+1)$ , and the product yield is denoted by  $f_{i(n)}^{j(n+1)}$ , as shown in Figure 1b. Obviously, the sum of  $f_{i(n)}^{j(n)}$  with respect to  $j(n)$  and the sum of  $f_{i(n)}^{j(n+1)}$  with respect to  $j(n+1)$  are unity. The feedstock composition and the product yield matrix are assumed to be known constants. The material flow from process to storage (or from storage to process) is represented by the PSW model, as shown in Figure 5. The material flow representation of the PSW model is composed of four variables: the batch size  $B_{i(n)}$ , the cycle time  $\omega_{i(n)}$ , the transportation time fraction  $x_{i(n)}^{(n+1)}$ , and the initial delay time  $t_{i(n)}^{j(n+1)}$ . The transportation time fraction is the fraction of transportation time over cycle time. The initial delay time is the first time at which the first batch is fed into or dispatched from the storage unit. The material flow of raw material purchased is represented by order size  $B_k^{j(1)}$ , cycle time  $\omega_k^{j(1)}$ , transportation time fraction  $x_k^{j(1)}$ , and initial delay time  $t_k^{j(1)}$ . All transportation time fractions will be considered as parameters of which the other will be the design variables used in this study. The material flow of finished product sales is represented by  $B_m^{j(N+1)}$ ,  $\omega_m^{j(N+1)}$ ,  $x_m^{j(N+1)}$ ,  $t_m^{j(N+1)}$  in the same

way. The arbitrary periodic function of the finished product demand forecast can be represented by the sum of periodic square wave functions with known values of  $B_m^{j(N+1)}$ ,  $\omega_m^{j(N+1)}$ ,  $x_m^{j(N+1)}$ ,  $t_m^{j(N+1)}$  (Yi and Reklaitis, 2000).

## Nonlinear Optimization Model of Plant Design

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 feed time, process time, and discharge time. In reality, there may exist sequences of feedstock feeding operations or product discharging operations, and the sequences depend upon the material transportation system design such as the pumping and piping network. Therefore, the material transportation 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 transportation facilities are not designed yet. Without loss of generality, 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 transportation time fractions are the same among feeding or discharging flows. That is, the superscript  $j$  is not necessary to discriminate the feedstock or product storage units under the following notations

$$t_{i(n)}^{j(n)} = t_{i(n)}^{(n)}, t_{i(n)}^{j(n+1)} = t_{i(n)}^{(n+1)}, x_{i(n)}^{j(n)} = x_{i(n)}^{(n)}, x_{i(n)}^{j(n+1)} = x_{i(n)}^{(n+1)} \quad (1)$$

Then, from the fact that one production cycle in a process is composed of feedstock feeding, processing, and product discharging, there exists the following timing relationship between the delay time of the feedstock stage and the delay time of the product stage

$$t_{i(n)}^{(n+1)} = t_{i(n)}^{(n)} + \omega_{i(n)}(1 - x_{i(n)}^{(n+1)}) \quad (2)$$

Let  $D_{i(n)}$  be the average material flow rate through process  $i(n)$ , which is batch size  $B_{i(n)}$  divided by cycle time  $\omega_{i(n)}$ . The average material flow through raw material storage, intermediate product storage, and finished product storage are denoted by  $D_k^{j(1)}$ ,  $D_{i(n)}^{j(n+1)}$ , and  $D_m^{j(N+1)}$ , respectively. The overall material balance around the storage results in the following relationships

$$D_{i(N+1)}^{j(N+1)} = \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} = \sum_{k=1}^{|kj(N+1)|} \frac{B_m^{j(N+1)}}{\omega_m^{j(N+1)}} \quad (3)$$

$$D_{i(n+1)}^{j(n+1)} = \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} = \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \quad (n=1, 2, \dots, N-1) \quad (4)$$

$$D_{i(1)}^{j(1)} = \sum_{k=1}^{|kj(1)|} D_k^{j(1)} = \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} \quad (5)$$

Suppose that the size of storage  $j(n+1)$  is denoted by  $V_s^{j(n+1)}$ , while the initial inventory of storage  $j(n+1)$  is denoted by  $V_s^{j(n+1)}(0)$ , and the inventory holdup of storage  $j(n+1)$  at time  $t$  is denoted by  $V_s^{j(n+1)}(t)$ . The inventory holdup can be calculated by the difference between the incoming

material flows from the supply processes and the outgoing material flows into the 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. The resulting inventory holdup functions for raw material, and intermediate and finished product storages are

$$V^{j(1)}(t) = V^{j(1)}(0) + \sum_{k=1}^{|kj(1)|} B_k^{j(1)} \left[ \text{int} \left[ \frac{t - t_k^{j(1)}}{\omega_k^{j(1)}} \right] + \min \left\{ 1, \frac{1}{x_k^{j(1)}} \text{res} \left[ \frac{t - t_k^{j(1)}}{\omega_k^{j(1)}} \right] \right\} \right] - \sum_{i=1}^{|i(1)|} (f_{i(1)}^{j(1)} B_{i(1)}) \times \left[ \text{int} \left[ \frac{t - t_{i(1)}^{(1)}}{\omega_{i(1)}} \right] + \min \left\{ 1, \frac{1}{x_{i(1)}^{(1)}} \text{res} \left[ \frac{t - t_{i(1)}^{(1)}}{\omega_{i(1)}} \right] \right\} \right] \quad (6)$$

$$V^{j(n+1)}(t) = V^{j(n+1)}(0) + \sum_{i=1}^{|i(n)|} (f_i^{j(n+1)} B_{i(n)}) \times \left[ \text{int} \left[ \frac{t - t_{i(n)}^{(n+1)}}{\omega_{i(n)}} \right] + \min \left\{ 1, \frac{1}{x_{i(n)}^{(n+1)}} \text{res} \left[ \frac{t - t_{i(n)}^{(n+1)}}{\omega_{i(n)}} \right] \right\} \right] - \sum_{i=1}^{|i(n+1)|} (f_{i(n+1)}^{j(n+1)} B_{i(n+1)}) \left[ \text{int} \left[ \frac{t - t_{i(n+1)}^{(n+1)}}{\omega_{i(n+1)}} \right] + \min \left\{ 1, \frac{1}{x_{i(n+1)}^{(n+1)}} \text{res} \left[ \frac{t - t_{i(n+1)}^{(n+1)}}{\omega_{i(n+1)}} \right] \right\} \right] \quad (7)$$

$$V^{j(N+1)}(t) = V^{j(N+1)}(0) + \sum_{i=1}^{|i(N)|} (f_{i(N)}^{j(N+1)} B_{i(N)}) \times \left[ \text{int} \left[ \frac{t - t_{i(N)}^{(N+1)}}{\omega_{i(N)}} \right] + \min \left\{ 1, \frac{1}{x_{i(N)}^{(N+1)}} \text{res} \left[ \frac{t - t_{i(N)}^{(N+1)}}{\omega_{i(N)}} \right] \right\} \right] - \sum_{m=1}^{|mj(N+1)|} B_m^{j(N+1)} \left[ \text{int} \left[ \frac{t - t_m^{j(N+1)}}{\omega_m^{j(N+1)}} \right] + \min \left\{ 1, \frac{1}{x_m^{j(N+1)}} \text{res} \left[ \frac{t - t_m^{j(N+1)}}{\omega_m^{j(N+1)}} \right] \right\} \right] \quad (8)$$

The upper bound of the inventory holdup, the lower bound of the inventory holdup, and the average inventory holdup of Eqs. 6–8 are calculated by using the properties of flow accumulation function, as can be seen in the Appendix.

$$V_{ub}^{j(1)} = V^{j(1)}(0) + \sum_{k=1}^{|kj(1)|} (1 - x_k^{j(1)}) D_k^{j(1)} \omega_k^{j(1)} - \sum_{k=1}^{|kj(1)|} D_k^{j(1)} t_k^{j(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{(1)} \quad (9)$$

$$V_{lb}^{j(1)} = V^{j(1)}(0) - \sum_{k=1}^{|kj(1)|} D_k^{j(1)} t_k^{j(1)} - \sum_{i=1}^{|i(1)|} (1 - x_{i(1)}^{(1)}) f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{(1)} \quad (10)$$

$$\overline{V^{j(1)}} = V^{j(1)}(0) + \sum_{k=1}^{|kj(1)|} \frac{(1 - x_k^{j(1)})}{2} D_k^{j(1)} \omega_k^{j(1)} - \sum_{k=1}^{|kj(1)|} D_k^{j(1)} t_k^{j(1)} - \sum_{i=1}^{|i(1)|} \frac{(1 - x_{i(1)}^{(1)})}{2} f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{(1)} \quad (11)$$

$$V_{ub}^{j(n+1)} = V^{j(n+1)}(0) + \sum_{i=1}^{|i(n)|} (1 - x_{i(n)}^{(n+1)}) f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} - \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \quad (12)$$

$$V_{lb}^{j(n+1)} = V^{j(n+1)}(0) - \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n+1)} - \sum_{i=1}^{|i(n+1)|} (1 - x_{i(n+1)}^{(n+1)}) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \quad (13)$$

$$\overline{V^{j(n+1)}} = V^{j(n+1)}(0) + \sum_{i=1}^{|i(n)|} \frac{(1 - x_{i(n)}^{(n+1)})}{2} f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} - \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n+1)} - \sum_{i=1}^{|i(n+1)|} \frac{(1 - x_{i(n+1)}^{(n+1)})}{2} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \quad (14)$$

$$V_{ub}^{j(N+1)} = V^{j(N+1)}(0) + \sum_{i=1}^{|i(N)|} (1 - x_{i(N)}^{(N+1)}) f_{i(N)}^{j(N+1)} D_{i(N)} \omega_{i(N)} - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} t_{i(N)}^{(N+1)} + \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} t_m^{j(N+1)} \quad (15)$$

$$V_{lb}^{j(N+1)} = V^{j(N+1)}(0) - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} t_{i(N)}^{(N+1)} - \sum_{m=1}^{|mj(N+1)|} (1 - x_m^{j(N+1)}) D_m^{j(N+1)} \omega_m^{j(N+1)} + \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} t_m^{j(N+1)} \quad (16)$$

$$\overline{V^{j(N+1)}} = V^{j(N+1)}(0) + \sum_{i=1}^{|i(N)|} \frac{(1 - x_{i(N)}^{(N+1)})}{2} f_{i(N)}^{j(N+1)} D_{i(N)} \omega_{i(N)} - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} t_{i(N)}^{(N+1)} - \sum_{m=1}^{|mj(N+1)|} \frac{(1 - x_m^{j(N+1)})}{2} D_m^{j(N+1)} \omega_m^{j(N+1)} + \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} t_m^{j(N+1)} \quad (17)$$

where Eq. 9 is the upper bound of raw material storage, Eq. 10 is the lower bound of raw material storage unit and Eq. 11

is the average inventory holdup of raw material storage unit. Equations 9–11 are derived from Eq. 6 by using the properties of PSW model as shown in the Appendix. Equations 12–14 are derived from Eq. 7 and Eqs. 15–17 are derived from Eq. 8. Note that  $n = 1, 2, \dots, N-1$  in Eq. 7 and Eqs. 12–14.

The purchasing setup cost of raw material  $j(1)$  is denoted by  $A_k^{j(1)}$  \$/order and the setup cost of process  $i(n)$  is denoted by  $A_{i(n)}$  \$/batch. The annual inventory holding cost of storage  $j(n)$  is denoted by  $H^{j(n)}$  \$/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. 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 analytical solution. The objective function for the design of the batch-storage network is to minimize the total cost consisted of the setup cost of processes, the inventory holding cost of storage units, and the capital cost of the processes and storage units.

$$TC = \sum_{j=1}^{|j(1)|} \sum_{k=1}^{|k(1)|} \left[ \frac{A_k^{j(1)}}{\omega_k^{j(1)}} + a_k^{j(1)} D_k^{j(1)} \omega_k^{j(1)} \right] + \sum_{n=1}^N \sum_{i=1}^{|i(n)|} \left[ \frac{A_{i(n)}}{\omega_{i(n)}} + a_{i(n)} D_{i(n)} \omega_{i(n)} \right] + \sum_{n=1}^{N+1} \sum_{j=1}^{|j(n)|} \left[ H^{j(n)} \overline{V^{j(n)}} + b^{j(n)} V_s^{j(n)} \right] \quad (18)$$

Where  $a_k^{j(1)}$  is the annual capital cost of the purchasing facility for raw material  $j(1)$ ,  $a_{i(n)}$  is the annual capital cost of process  $i(n)$ , and  $b^{j(n)}$  is the capital cost of storage  $j(n)$ . Without loss of generality, the storage size  $V_s^{j(n+1)}$  will be determined by the upper bound of inventory holdup,  $V_{ub}^{j(n+1)}$ . Therefore, Eqs. 9, 12, and 15 are the expressions for storage capacities. The independent variables are selected to be the cycle times  $\omega_k^{j(1)}$ ,  $\omega_{i(n)}$ , initial time delays  $t_k^{j(1)}$ ,  $t_{i(n)}^{(n)}$ , and average material flow rates  $D_k^{j(1)}$ ,  $D_{i(n)}$ . The initial time delay  $t_{i(n)}^{(n+1)}$  is converted into  $t_{i(n)}^{(n)}$  by Eq. 2. Equation 18 can be transformed into the following expression in terms of the independent variables by using Eqs. 2, 9, 11, 12, 14, 15, and 17

$$TC = \sum_{j=1}^{|j(1)|} \sum_{k=1}^{|k(1)|} \left[ \frac{A_k^{j(1)}}{\omega_k^{j(1)}} \right] + \sum_{n=1}^N \sum_{i=1}^{|i(n)|} \left[ \frac{A_{i(n)}}{\omega_{i(n)}} \right] + \sum_{j=1}^{|j(1)|} \sum_{k=1}^{|k(1)|} \left[ \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) (1 - x_k^{j(1)}) + a_k^{j(1)} \right] D_k^{j(1)} \omega_k^{j(1)} - \sum_{j=1}^{|j(1)|} \sum_{k=1}^{|k(1)|} (H^{j(1)} + b^{j(1)}) D_k^{j(1)} t_k^{j(1)} + \sum_{n=1}^N \sum_{i=1}^{|i(n)|} a_{i(n)} D_{i(n)} \omega_{i(n)} - \sum_{n=1}^N \sum_{i=1}^{|i(n)|} \left[ (1 - x_{i(n)}^{(n)}) \sum_{j=1}^{|j(n)|} f_{i(n)}^{j(n)} \left( \frac{H^{j(n)}}{2} \right) + (1 - x_{i(n)}^{(n+1)}) \sum_{j=1}^{|j(n+1)|} f_{i(n)}^{j(n+1)} \left( \frac{H^{j(n+1)}}{2} \right) \right] D_{i(n)} \omega_{i(n)} \quad (19)$$

$$+ \sum_{n=1}^N \sum_{i=1}^{|i(n)|} \left[ \sum_{j=1}^{|j(n)|} f_{i(n)}^{j(n)} (H^{j(n)} + b^{j(n)}) - \sum_{j=1}^{|j(n+1)|} f_{i(n)}^{j(n+1)} (H^{j(n+1)} + b^{j(n+1)}) \right] D_{i(n)} t_{i(n)}^{(n)} + \text{constants} \quad (19)$$

where constants are

$$\text{constants} = \sum_{n=1}^{N+1} \sum_{j=1}^{|j(1)|} (H^{j(n)} + b^{j(n)}) V^{j(n)}(0) - \sum_{j=1}^{|j(N+1)|} \sum_{m=1}^{|mj(N+1)|} \left( \frac{H^{j(N+1)}}{2} \right) (1 - x_m^{j(N+1)}) D_m^{j(N+1)} \omega_m^{j(N+1)} + \sum_{j=1}^{|j(N+1)|} \sum_{m=1}^{|mj(N+1)|} (H^{j(N+1)} + b^{j(N+1)}) D_m^{j(N+1)} t_m^{j(N+1)} \quad (20)$$

The inventory holdup  $V^{j(n)}(t)$  should be confined within the storage capacity. Sufficient conditions are  $0 \leq V_{lb}^{j(n)} < V_{ab}^{j(n)} \leq V_s^{j(n)}$ . Since the storage size  $V_s^{j(n)}$  should be determined through this analysis, only the conditions  $0 \leq V_{lb}^{j(n)}$  are necessary. The lower bounds of holdup Eqs. 10, 13, and 16 are given by the following inequalities

$$V^{j(1)}(0) - \sum_{k=1}^{|k(1)|} D_k^{j(1)} t_k^{j(1)} - \sum_{i=1}^{|i(1)|} (1 - x_{i(1)}^{(1)}) f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{(1)} \geq 0 \quad (21)$$

$$V^{j(n+1)}(0) - \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n)} - \sum_{i=1}^{|i(n)|} (1 - x_{i(n)}^{(n+1)}) f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} - \sum_{i=1}^{|i(n+1)|} (1 - x_{i(n+1)}^{(n+1)}) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \geq 0 \quad (n = 1, 2, \dots, N-1) \quad (22)$$

$$V^{j(N+1)}(0) - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} t_{i(N)}^{(N)} - \sum_{i=1}^{|i(N)|} (1 - x_{i(N)}^{(N+1)}) f_{i(N)}^{j(N+1)} D_{i(N)} \omega_{i(N)} - \sum_{m=1}^{|mj(N+1)|} (1 - x_m^{j(N+1)}) D_m^{j(N+1)} \omega_m^{j(N+1)} + \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} t_m^{j(N+1)} \geq 0 \quad (23)$$

The problem is defined as minimizing the total cost given by Eq. 19 subject to the constraints of Eqs. 3–5 and 21–23 with respect to the non-negative search variables  $\omega_k^{j(1)}$ ,  $\omega_{i(n)}$ ,  $t_k^{j(1)}$ ,  $t_{i(n)}^{(n)}$  and  $D_k^{j(1)}$ ,  $D_{i(n)}$ . All of  $D_{i(n)}$  can be excluded from independent variables when the product yield matrix  $f_{i(n)}^{j(n+1)}$  is square and invertible, because they are directly determined by Eqs. 3–5. The objective function (Eq. 19) is convex and the constants are linear with respect to  $\omega_k^{j(1)}$ ,  $\omega_{i(n)}$  and  $t_k^{j(1)}$ ,  $t_{i(n)}^{(n)}$  if  $D_k^{j(1)}$ ,  $D_{i(n)}$  are considered as parameters. However, the convexity about  $D_k^{j(1)}$ ,  $D_{i(n)}$  is not clear. At first, we will show that the Kuhn-Tucker conditions with respect to  $\omega_k^{j(1)}$ ,  $\omega_{i(n)}$  and  $t_k^{j(1)}$ ,  $t_{i(n)}^{(n)}$  push the Eqs. 21, 22, and 23 into equalities and, then, we will examine the convexity of the resulting objective function with respect to  $D_k^{j(1)}$ ,  $D_{i(n)}$  after eliminating the other variables.

### Solution of Kuhn-Tucker Conditions

The Lagrange multipliers for constraints of Eqs. 3–5 and Eqs. 21–23 are denoted  $\lambda_D^{j(N+1)}$ ,  $\lambda_D^{j(n+1)}$ ,  $\lambda_D^{j(1)}$  and  $\lambda_{lb}^{j(n+1)}$ ,  $\lambda_{lb}^{j(n+1)}$ , respectively. Here,  $\lambda_{lb}^{j(1)}$ ,  $\lambda_{lb}^{j(n+1)}$ ,  $\lambda_{lb}^{j(N+1)}$  are required to take on non-negative values. We will add two more terms resulted from the conditions  $D_k^{j(1)} \geq 0$  and  $D_{i(n)} \geq 0$  to the Lagrangian for the mathematical consistency. The corresponding Lagrange multipliers are  $\lambda_k^{j(1)}$ ,  $\lambda_{i(n)} \geq 0$  respectively. The resulting Lagrangian is

$$\begin{aligned}
 L = TC & - \sum_{j=1}^{|j(N+1)|} \lambda_D^{j(N+1)} \left[ \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} - D^{j(N+1)} \right] \\
 & - \sum_{n=1}^{N-1} \sum_{j=1}^{|j(n+1)|} \lambda_D^{j(n+1)} \left[ \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} \right. \\
 & \quad \left. - \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \right] \\
 & - \sum_{j=1}^{|j(1)|} \lambda_D^{j(1)} \left[ \sum_{k=1}^{|k(1)|} D_k^{j(1)} - \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} \right] \\
 & - \sum_{j=1}^{|j(1)|} \lambda_{lb}^{j(1)} \left[ V^{j(1)}(0) - \sum_{k=1}^{|k(1)|} D_k^{j(1)} t_k^{j(1)} \right. \\
 & \quad \left. - \sum_{i=1}^{|i(1)|} (1 - x_{i(1)}^{(1)}) f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{(1)} \right] \\
 & - \sum_{n=1}^{N-1} \sum_{j=1}^{|j(n+1)|} \lambda_{lb}^{j(n+1)} \left[ V^{j(n+1)}(0) - \sum_{i=1}^{|i(n)|} \right. \\
 & \quad \times f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \\
 & \quad \left. - \sum_{i=1}^{|i(n)|} (1 - x_{i(n)}^{(n+1)}) f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} \right. \\
 & \quad \left. - \sum_{i=1}^{|i(n+1)|} (1 - x_{i(n+1)}^{(n+1)}) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} \right]
 \end{aligned}$$

$$\begin{aligned}
 & - \sum_{j=1}^{|j(N+1)|} \lambda_{lb}^{j(N+1)} \left[ V^{j(N+1)}(0) - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} \right. \\
 & \quad \times D_{i(N)} t_{i(N)}^{(N)} + \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} t_m^{j(N+1)} \\
 & \quad - \sum_{i=1}^{|i(N)|} (1 - x_{i(N)}^{(N+1)}) f_{i(N)}^{j(N+1)} D_{i(N)} \omega_{i(N)} \\
 & \quad \left. - \sum_{m=1}^{|mj(N+1)|} (1 - x_m^{(N+1)}) D_m^{j(N+1)} \omega_m^{j(N+1)} \right] \quad (24) \\
 & - \sum_{j=1}^{|j(1)|} \sum_{k=1}^{|k(1)|} \lambda_k^{j(1)} D_k^{j(1)} - \sum_{n=1}^N \sum_{i=1}^{|i(n)|} \lambda_{i(n)} D_{i(n)}
 \end{aligned}$$

Kuhn-Tucker conditions result in the following equations (Reklaitis et al., 1983)

$$\frac{\partial L}{\partial t_k^{j(1)}} = -(H^{j(1)} + b^{j(1)}) D_k^{j(1)} + \lambda_{lb}^{j(1)} D_k^{j(1)} = 0 \quad (25)$$

$$\begin{aligned}
 \frac{\partial L}{\partial \omega_k^{j(1)}} &= -\frac{A_k^{j(1)}}{(\omega_k^{j(1)})^2} \\
 &+ \left[ \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) (1 - x_k^{j(1)}) + a_k^{j(1)} \right] D_k^{j(1)} = 0 \quad (26)
 \end{aligned}$$

$$\begin{aligned}
 D_k^{j(1)} \left[ \omega_k^{j(1)} \left[ \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) (1 - x_k^{j(1)}) + a_k^{j(1)} \right] \right. \\
 \left. - (H^{j(1)} + b^{j(1)}) t_k^{j(1)} + \lambda_{lb}^{j(1)} t_k^{j(1)} - \lambda_k^{j(1)} - \lambda_D^{j(1)} \right] = 0 \quad (27)
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial L}{\partial t_{i(n)}^{(n)}} &= \left[ \sum_{j=1}^{|j(n)|} (H^{j(n)} + b^{j(n)}) f_{i(n)}^{j(n)} \right. \\
 & \quad \left. - \sum_{j=1}^{|j(n+1)|} (H^{j(n+1)} + b^{j(n+1)}) f_{i(n)}^{j(n+1)} \right] D_{i(n)} \\
 & - \left[ \sum_{j=1}^{|j(n)|} \lambda_{lb}^{j(n)} f_{i(n)}^{j(n)} - \sum_{j=1}^{|j(n+1)|} \lambda_{lb}^{j(n+1)} f_{i(n)}^{j(n+1)} \right] D_{i(n)} = 0 \\
 & \quad (n = 1, 2, \dots, N) \quad (28)
 \end{aligned}$$

$$\begin{aligned}
 \frac{\partial L}{\partial \omega_{i(n)}} &= -\frac{A_{i(n)}}{(\omega_{i(n)})^2} + a_{i(n)} D_{i(n)} \\
 & - \left\{ (1 - x_{i(n)}^{(n)}) \sum_{j=1}^{|j(n)|} \left( \frac{H^{j(n)}}{2} \right) f_{i(n)}^{j(n)} + (1 - x_{i(n)}^{(n+1)}) \right. \\
 & \quad \times \sum_{j=1}^{|j(n+1)|} \left( \frac{H^{j(n+1)}}{2} \right) f_{i(n)}^{j(n+1)} \Big\} D_{i(n)} \\
 & + \left\{ (1 - x_{i(n)}^{(n)}) \sum_{j=1}^{|j(n)|} \lambda_{lb}^{j(n)} f_{i(n)}^{j(n)} + (1 - x_{i(n)}^{(n+1)}) \right. \\
 & \quad \times \sum_{j=1}^{|j(n+1)|} \lambda_{lb}^{j(n+1)} f_{i(n)}^{j(n+1)} \Big\} D_{i(n)} = 0 \quad (n = 1, 2, \dots, N) \quad (29)
 \end{aligned}$$



$$Di(n) \left[ - \left\{ \left( 1 - x_{i(n)}^{(n)} \right) \sum_{j=1}^{|j(n)|} \left( \frac{H^{j(n)}}{2} \right) f_{i(n)}^{j(n)} + \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} t_m^{j(N+1)} \right\} = 0 \quad (33)$$

$$+ \left( 1 - x_{i(n)}^{(n+1)} \right) \sum_{j=1}^{|j(n+1)|} \left( \frac{H^{j(n+1)}}{2} \right) f_{i(n)}^{j(n+1)} \right\} \omega_{i(n)}$$

$$+ \left\{ \left( 1 - x_{i(n)}^{(n)} \right) \sum_{j=1}^{|j(n)|} \lambda_{lb}^{j(n)} f_{i(n)}^{j(n)} \right.$$

$$+ \left( 1 - x_{i(n)}^{(n+1)} \right) \sum_{j=1}^{|j(n+1)|} \lambda_{lb}^{j(n+1)} f_{i(n)}^{j(n+1)} \left. \right\} \omega_{i(n)}$$

$$+ \left[ \sum_{j=1}^{|j(n)|} (H^{j(n)} + b^{j(n)}) f_{i(n)}^{j(n)} - \sum_{j=1}^{|j(n+1)|}$$

$$\times (H^{j(n+1)} + b^{j(n+1)}) f_{i(n)}^{j(n+1)} \right] t_{i(n)}^{(n)}$$

$$- \left[ \sum_{j=1}^{|j(n)|} \lambda_{lb}^{j(n)} f_{i(n)}^{j(n)} - \sum_{j=1}^{|j(n+1)|} \lambda_{lb}^{j(n+1)} f_{i(n)}^{j(n+1)} \right] t_{i(n)}^{(n)}$$

$$+ \sum_{j=1}^{|j(n)|} \lambda_D^{j(n)} f_{i(n)}^{j(n)} - \sum_{j=1}^{|j(n+1)|} \lambda_D^{j(n+1)} f_{i(n)}^{j(n+1)}$$

$$- \lambda_{i(n)} + a_{i(n)} \omega_{i(n)} \left. \right] = 0 \quad (n = 1, 2, \dots, N) \quad (30)$$

$$\lambda_{lb}^{j(1)} \left[ V^{j(1)}(0) - \sum_{k=1}^{|kj(1)|} D_k^{j(1)} t_k^{j(1)} - \sum_{i=1}^{|i(1)|} \left( 1 - x_{i(1)}^{(1)} \right) f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{(1)} \right] = 0 \quad (31)$$

$$\lambda_{lb}^{j(n+1)} \left[ V^{j(n+1)}(0) - \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n)} - \sum_{i=1}^{|i(n)|} \left( 1 - x_{i(n)}^{(n+1)} \right) f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} - \sum_{i=1}^{|i(n+1)|} \left( 1 - x_{i(n+1)}^{(n+1)} \right) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \right] = 0 \quad (n = 1, 2, \dots, N-1) \quad (32)$$

$$\lambda_{lb}^{j(N+1)} \left[ V^{j(N+1)}(0) - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} t_{i(N)}^{(N)} - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} \left( 1 - x_{i(N)}^{(N+1)} \right) D_{i(N)} \omega_{i(N)} - \sum_{m=1}^{|mj(N+1)|} \left( 1 - x_m^{(N+1)} \right) D_m^{j(N+1)} \omega_m^{j(N+1)} \right]$$

Solving Eq. 25 gives

$$\lambda_{lb}^{j(1)} = H^{j(1)} + b^{j(1)} \quad (34)$$

Solving Eq. 26 gives

$$\omega_k^{j(1)} = \sqrt{\frac{A_k^{j(1)}}{D_k^{j(1)} \left[ \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) \left( 1 - x_k^{j(1)} \right) + a_k^{j(1)} \right]}} \quad (35)$$

Solving Eq. 28 gives

$$\lambda_{lb}^{j(n)} = H^{j(n)} + b^{j(n)} \quad (36)$$

Equation 29 can be resolved with respect to  $\omega_{i(n)}$  after removing some terms by inserting Eq. 36 into it

$$\omega_{i(n)} = \sqrt{\frac{A_{i(n)}}{D_{i(n)} \Psi_{i(n)}}} \quad (n = 1, 2, \dots, N) \quad (37)$$

where

$$\Psi_{i(n)} = a_{i(n)} + \left( 1 - x_{i(n)}^{(n)} \right) \sum_{j=1}^{|j(n)|} \left( \frac{H^{j(n)}}{2} + b^{j(n)} \right) f_{i(n)}^{j(n)} + \left( 1 - x_{i(n)}^{(n+1)} \right) \sum_{j=1}^{|j(n+1)|} \left( \frac{H^{j(n+1)}}{2} + b^{j(n+1)} \right) f_{i(n)}^{j(n+1)} \quad (38)$$

Equation 38 indicates that the inventory holding costs of all storage units connected to a process influence the optimal lot size of the process.

Since all the Lagrange multipliers are positive from Eqs. 34 and 36, the initial delay times can be derived from Eqs. 31–33

$$\sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} D_{i(N)} t_{i(N)}^{(N)} = V^{j(N+1)}(0) - \sum_{m=1}^{|mj(N+1)|} \left( 1 - x_m^{(N+1)} \right) D_m^{j(N+1)} \omega_m^{j(N+1)} + \sum_{m=1}^{|mj(N+1)|} \left( 1 - x_m^{(N+1)} \right) D_m^{j(N+1)} \omega_m^{j(N+1)} \times D_m^{j(N+1)} t_m^{j(N+1)} - \sum_{i=1}^{|i(N)|} f_{i(N)}^{j(N+1)} \left( 1 - x_{i(N)}^{(N+1)} \right) D_{i(N)} \omega_{i(N)} \quad (39)$$

$$\sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n)} = V^{j(n+1)}(0) - \sum_{i=1}^{|i(n+1)|} \left( 1 - x_{i(n+1)}^{(n+1)} \right) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} - \sum_{i=1}^{|i(n)|} \left( 1 - x_{i(n)}^{(n+1)} \right) \times f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} \quad (n = 1, 2, \dots, N-1) \quad (40)$$

$$\sum_{k=1}^{|kj(1)|} D_k^{j(1)} t_k^{j(1)} = V^{j(1)}(0) - \sum_{i=1}^{|i(1)|} (1 - x_{i(1)}^{j(1)}) f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} + \sum_{i=1}^{|i(1)|} f_{i(1)}^{j(1)} D_{i(1)} t_{i(1)}^{j(1)} \quad (41)$$

Note that Eqs. 39 and 40 give  $|j(n+1)|$  equations and  $|i(n)|$  unknowns for each stage with respect to the initial delay times. Equation 41 gives  $|j(1)|$  equations and  $|j(1)| \times |kj(1)|$  unknowns. This additional freedom with respect to the initial delay times will be removed after Proposition II.

The minimum value of the objective function Eq. 19 obtained at the optimal solution Eqs. 35, 37, and 39–41 is

$$\begin{aligned} *TC(D_k^{j(1)}, D_{i(n)}) &= 2 \sum_{j=1}^{|j(1)|} \sum_{k=1}^{|kj(1)|} \sqrt{A_k^{j(1)} \left[ (1 - x_k^{j(1)}) \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) + a_k^{j(1)} \right] D_k^{j(1)}} \\ &\quad + 2 \sum_{n=1}^N \sum_{i=1}^{|i(n)|} \sqrt{D_{i(n)} A_{i(n)} \Psi_{i(n)}} \\ &\quad + \sum_{j=1}^{|j(N+1)|} \left( \frac{H^{j(N+1)}}{2} + b^{j(N+1)} \right) \sum_{m=1}^{|mj(N+1)|} \\ &\quad \times D_m^{j(N+1)} \omega_m^{j(N+1)} (1 - x_m^{j(N+1)}) \quad (42) \end{aligned}$$

### Global Minimum Point of Concave Objective Function

The objective function of Eq. 42 is not optimized with respect to  $D_k^{j(1)}$ ,  $D_{i(n)}$ . Unfortunately, the relevant Kuhn-Tucker conditions (Eqs. 27 and 30) are not helpful because the objective function (Eq. 42) is concave with respect to  $D_k^{j(1)}$ ,  $D_{i(n)}$ . To consider these, we will take an indirect approach. We will introduce some terminology and some reasonable assumptions in order to find the global minimum.

Let  $I(n)$  ( $I = 1, 2, \dots, |I(n)|$ ) be the sets of processes with the same product yield where  $|I(n)| = |j(n+1)|$ . The processes in set  $I(n)$  can be considered as a single process, because they produce the same ratio of products. The intermediate product average consumption rate with respect to the process group set  $I(n)$  ( $D_{I(n)}$ ) is the sum of individual product consumption rate of the process in set  $I(n)$

$$D_{I(n)} = \sum_{i(n) \in I(n)} D_{i(n)} \quad (n = 1, 2, \dots, N) \quad (43)$$

**Proposition I.** When  $|i(n)| > |j(n+1)|$ ,  $D^{j(n)}$  can be calculated from  $D^{j(n+1)}$  if the following conditions hold for  $n = N, N-1, \dots, 1$ .

$$(i) \det(f_{i(n)}^{j(n+1)}) \neq 0$$

$$(ii) f_{i_1(n)}^{j(n)} = f_{i_2(n)}^{j(n)}, \text{ for } i_1(n), i_2(n) \text{ such that}$$

$$f_{i_1(n)}^{j(n+1)} = f_{i_2(n)}^{j(n+1)} \quad (44)$$

$$(iii) D_{I(n)} = \frac{\sum_{j=1}^{|j(n+1)|} D^{j(n+1)} * \text{cofactor of } (f_{I(n)}^{j(n+1)})}{\det(f_{I(n)}^{j(n+1)})} > 0$$

**Proof.** Suppose that the processes with the same product yield have the same feedstock composition, that is,  $f_{i_1(n)}^{j(n)} = f_{i_2(n)}^{j(n)}$  for  $i_1(n), i_2(n) \in I(n)$ . Then, Eq. 4 can be grouped by set  $I(n)$ .  $D_{I(n)}$  replaces the sum of  $D_{i(n)}$  with respect to  $i(n) \in I(n)$ . Because the product yield matrix  $f_{I(n)}^{j(n+1)}$  is invertible,  $D_{I(n)}$  can be calculated from  $D^{j(n+1)}$  by using Eq. 4. Also  $D^{j(n)}$  can be calculated from  $D_{I(n)}$  by using Eq. 4 because the processes in set  $I(n)$  have the same feedstock composition. The condition (iii) comes from  $D_{I(n)} > 0$  where  $D_{I(n)}$  is calculated by Cramer's rule.

The meaning of the first condition of Eq. 44 is that the number of process groups with a different product yield should be equal to the number of products. When the number of process groups with a different product yield is less than the number of products, Eqs. 3–5 cannot be satisfied. In this case, the number of considered products should be reduced to the number of process groups with a different product yield. When the number of process groups with different product yield is greater than the number of products, Eqs. 3–5 cannot be satisfied, as well. In this case, the number of process groups considered should be reduced to the number of products. Even though the number of processes are greater than the number of products, if some processes have the same product yield and the number of process groups with different product yield are still equal to the number of products,  $D^{j(n)}$  can be calculated from  $D^{j(n+1)}$  under the condition that the feedstock composition is the same for the process groups with the same product yield. 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 limit which originates from technical and/or safety concern. In this article, the process is characterized by the parameters of feedstock composition, product yield, transportation 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 transportation time fraction, setup cost, and capital cost, called similar processes and need additional analysis.

Under the assumptions of Eq. 44, Eqs. 3–5 are solved for all  $D_k^{j(1)}$ ,  $D_{i(n)}$  resulting in Eq. 43 and the following equation

$$\sum_{k=1}^{|kj(1)|} D_k^{j(1)} = D^{j(1)} \quad (45)$$

The objection function (Eq. 42) and the constraints (Eqs. 43 and 45) constitute a new optimization problem with respect to  $D_k^{j(1)}$ ,  $D_{i(n)}$ . The optimization problem can be completely segregated into two parts with respect to variables  $D_k^{j(1)}$  and variables  $D_{i(n)}$ . The two parts of the optimization problem have the same formulation and the resulting solution is summarized as Proposition II.

**Proposition II.** Suppose  $\alpha_p$  ( $p = 1, 2, \dots, P$ ) are positive constants. The optimal solution of  $\min_{z_p} \sum_{p=1}^P \alpha_p \sqrt{z_p}$  under the constraints  $\sum_{p=1}^P z_p = Z$  and  $z_p \geq 0$  is  $z_{p^*} = Z$  and  $z_p = 0$  for  $p \neq p^*$  with the optimal objective value of  $\min_p \alpha_p \sqrt{Z}$  where  $p^*$  is selected to be the minimum.

**Proof.** All feasible variables are confined within a hyperplane  $C = \{z_p | \sum_{p=1}^P z_p = Z \text{ and } z_p \geq 0\}$ . The last variable can be removed by  $z_p = Z - \sum_{p=1}^{P-1} z_p$ . The objective function becomes  $\sum_{p=1}^{P-1} \alpha_p \sqrt{z_p} + \alpha_P \sqrt{Z - \sum_{p=1}^{P-1} z_p}$ . For any arbitrary two points  $z_p^1, z_p^2 \in C$  and  $0 \leq \delta \leq 1$ , the Jensen's inequality provides

$$\begin{aligned} \sum_{p=1}^{P-1} \alpha_p \sqrt{\delta z_p^1 + (1-\delta)z_p^2} &\geq \sum_{p=1}^{P-1} \alpha_p \left( \delta \sqrt{z_p^1} + (1-\delta) \sqrt{z_p^2} \right) \\ &= \delta \sum_{p=1}^{P-1} \alpha_p \sqrt{z_p^1} + (1-\delta) \sum_{p=1}^{P-1} \alpha_p \sqrt{z_p^2} \\ &\quad \times \alpha_P \sqrt{Z - \sum_{p=1}^{P-1} (\delta z_p^1 + (1-\delta)z_p^2)} \\ &= \alpha_P \sqrt{\delta \left( Z - \sum_{p=1}^{P-1} z_p^1 \right) + (1-\delta) \left( Z - \sum_{p=1}^{P-1} z_p^2 \right)} \\ &\geq \alpha_P \left[ \delta \sqrt{Z - \sum_{p=1}^{P-1} z_p^1} + (1-\delta) \sqrt{Z - \sum_{p=1}^{P-1} z_p^2} \right] \end{aligned}$$

Where the equalities hold when  $z_p^1 = z_p^2$ . Therefore, the objective function is strictly concave for any positive integer  $P$ . Partial differentiation of the objective function gives

$$z_p^* = \left( \frac{Z}{\sum_{p=1}^P \left( \frac{1}{\alpha_p} \right)^2} \right) \left( \frac{1}{\alpha_p} \right)^2 \quad (46)$$

Equation 46 indicates that the stationary point  $z_p^*$ , which is the maximum of the concave objective function, is unique and exists strictly inside of the hyperplane  $C$ . The optimum (minimum) point must be on the boundary of the hyperplane  $C$  and, therefore, at least one of the variables is zero at the optimum point. This statement is true for any positive integer of  $P$ . If we apply this statement one by one, we can reduce the number of possible nonzero variables, and at last, one variable  $z_{p^*} = Z$  will remain. Therefore, the optimum point consists of one nonzero variable and all the other zero variables. The global optimum point will be selected such that the optimum value is  $\min_p \alpha_p \sqrt{Z}$ .

Proposition II suggests that only one of the average material flow rates in Eqs. 43 and 45 is nonzero and all the others are zero at the optimum point

$$D_{i(n)^*} = D_{l(n)}, D_{k^*}^{j(1)} = D^{j(1)} \quad (47)$$

where  $i(n)^*$  is selected from the minimum of  $A_{i(n)} \Psi_{i(n)}$  among set  $l(n)$  and  $k^*$  is selected from the minimum of

$$A_k^{j(1)} \left[ \left( 1 - x_k^{j(1)} \right) \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) + \alpha_k^{j(1)} \right]$$

Equation 47 satisfies the Kahn-Tucker conditions (Eqs. 27 and 30). The corresponding optimum value of the objective function is

$$\begin{aligned} {}^*TC &= 2 \sum_{j=1}^{|j(1)|} \sqrt{\min_k \left\{ A_k^{j(1)} \left[ \left( 1 - x_k^{j(1)} \right) \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) + \alpha_k^{j(1)} \right] \right\} D^{j(1)}} \\ &\quad + 2 \sum_{n=1}^N \sum_{l=1}^{|l(n)|} \sqrt{\min_{i(n) \in l(n)} \{ A_{i(n)} \Psi_{i(n)} \} D_{l(n)}} \\ &\quad + \sum_{j=1}^{|j(N+1)|} \left( \frac{H^{j(N+1)}}{2} + b^{j(N+1)} \right) \\ &\quad \times \sum_{m=1}^{|mj(N+1)|} D_m^{j(N+1)} \omega_m^{j(N+1)} (1 - x_m^{j(N+1)}) \quad (48) \end{aligned}$$

After calculating all  $D_k^{j(1)}$ ,  $D_{i(n)}$ , the optimal cycle times are calculated by Eqs. 35 and 37 and, therefore, the optimal batch sizes can be determined. Finally, inserting Eqs. 39–41 into Eqs. 9, 12, and 15 gives the optimal storage size

$$\begin{aligned} {}^*V_s^{j(1)} &= \sum_{k=1}^{|kj(1)|} (1 - x_k^{j(1)}) D_k^{j(1)} \omega_k^{j(1)} \\ &\quad + \sum_{i=1}^{|i(1)|} (1 - x_{i(1)}^{(1)}) f_{i(1)}^{j(1)} D_{i(1)} \omega_{i(1)} \quad (49) \end{aligned}$$

$$\begin{aligned} {}^*V_s^{j(n+1)} &= \sum_{i=1}^{|i(n)|} (1 - x_{i(n)}^{(n+1)}) f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} \\ &\quad + \sum_{i=1}^{|i(n+1)|} (1 - x_{i(n+1)}^{(n+1)}) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} \\ &\quad (n = 1, 2, \dots, N-1) \quad (50) \end{aligned}$$

$$\begin{aligned} {}^*V_s^{j(N+1)} &= \sum_{i=1}^{|i(N)|} (1 - x_{i(N)}^{(N+1)}) f_{i(N)}^{j(N+1)} D_{i(N)} \omega_{i(N)} \\ &\quad + \sum_{m=1}^{|mj(N+1)|} (1 - x_m^{(N+1)}) D_m^{j(N+1)} \omega_m^{j(N+1)} \quad (51) \end{aligned}$$

## Optimal Design Procedure

From the results of the above optimization solution, the optimal design procedure for the batch-storage network is summarized as follows:

(1) Arrange the processes and storage units in the network structure as shown in Figure 3. If it is necessary, insert dummy processes and/or storage units, which have no capacity and no time delay. Serial processes without storage can be considered as one process. The storage units containing the same material should be considered as one storage unit. If the number of processes is less than the number of products, aggregate some of the products. Calculate all average material flow rates passing through the processes and storages by using Eqs. 3–5. Choose only one process that has the minimum value of  $A_{i(n)}\Psi_{i(n)}$  among similar processes. Average material flow rates can be determined by other methods such as linear programming and can be considered as fixed parameters without affecting the optimality.

(2) Identify all storage units connected to the process  $i$  under construction as shown at Figure 6. Here  $j(1)$  represents the feedstock storage unit and  $j(2)$  represents the product storage unit. Prepare the necessary input data such as feedstock composition, product yield, transportation time fractions, setup cost, inventory holding costs, capital costs and average material flow rates. The optimal batch size of process  $i$  is calculated by the following equation derived from Eq. 37.

$$^*B_i = \sqrt{\frac{A_i D_i}{a_i + (1 - x_i^{(1)}) \sum_{j=1}^{|j(1)|} \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) f_i^{j(1)} + (1 - x_i^{(2)}) \sum_{j=1}^{|j(2)|} \left( \frac{H^{j(2)}}{2} + b^{j(2)} \right) f_i^{j(2)}}} \quad (52)$$

The optimal lot size for raw material purchase is calculated by Eq. 35 and only one supplier  $k$  that has the minimum value of

$$A_k^{j(1)} \left[ (1 - x_k^{j(1)}) \left( \frac{H^{j(1)}}{2} + b^{j(1)} \right) + a_k^{j(1)} \right]$$

should be selected.

(3) Identify all processes connected to the storage  $j$ , as shown at Figure 7. Subscript  $i(1)$  represents the supply process and  $i(2)$  represents the consumption process. The initial delay times of each stage are sequentially calculated from the finished product delivery time of the final stage using the following equation derived from Eqs. 39–41.

$$\sum_{i=1}^{|i(1)|} D_{i(1)}^j t_{i(1)}^j - \sum_{i=1}^{|i(2)|} D_{i(2)}^j t_{i(2)}^j = V^j(0) - \sum_{i=1}^{|i(2)|} B_{i(2)}^j (1 - x_{i(2)}^j) \quad (53)$$

where  $D_{i(1)}^j$ ,  $D_{i(2)}^j$  are the average material flow rate between storage  $j$  and processes  $i(1)$  or  $i(2)$  and, that is,  $D_{i(1)}^j = D_{i(1)} f_{i(1)}^j$ ,  $D_{i(2)}^j = D_{i(2)} f_{i(2)}^j$ . Also,  $B_{i(2)}^j$  is the batch size of the consumption processes, that is,  $B_{i(2)}^j = B_{i(2)} f_{i(2)}^j$ . The optimal size of storage  $j$  is calculated by the following equation derived from Eqs. 49–51.

$$^*V_s^j = \sum_{i=1}^{|i(1)|} (1 - x_{i(1)}^j) B_{i(1)}^j + \sum_{i=1}^{|i(2)|} (1 - x_{i(2)}^j) B_{i(2)}^j \quad (54)$$

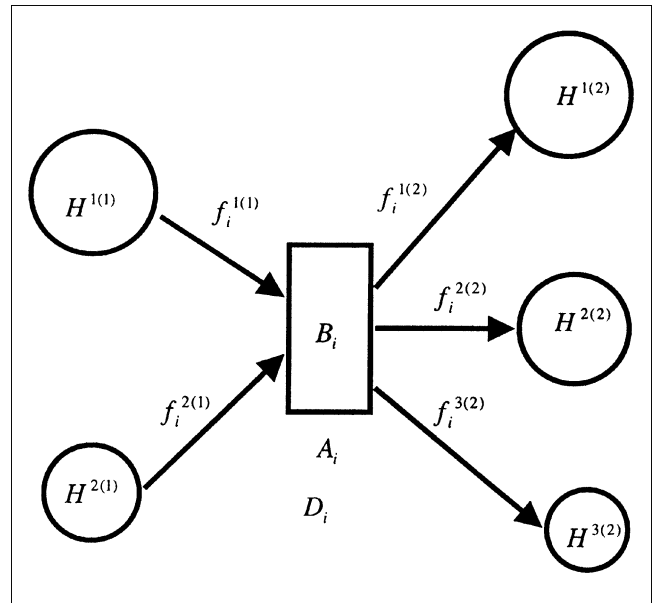


Figure 6. Optimal size of batch process connected by storage.

## Example Plant Design and Discussions

Consider a plant that produces three finished products from four raw materials, as shown in Figure 8. The plant is composed of three stages. The first stage has four raw material storage units and two processes. The second stage has two storage units and three processes. The third stage has three finished product storage units. The customer demands of finished products are assumed to be constant for convenience,

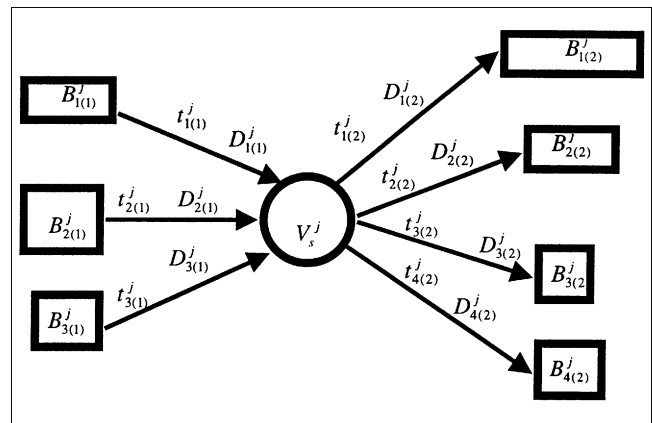


Figure 7. Optimal size of storage connected by multiple supply and consumption processes.

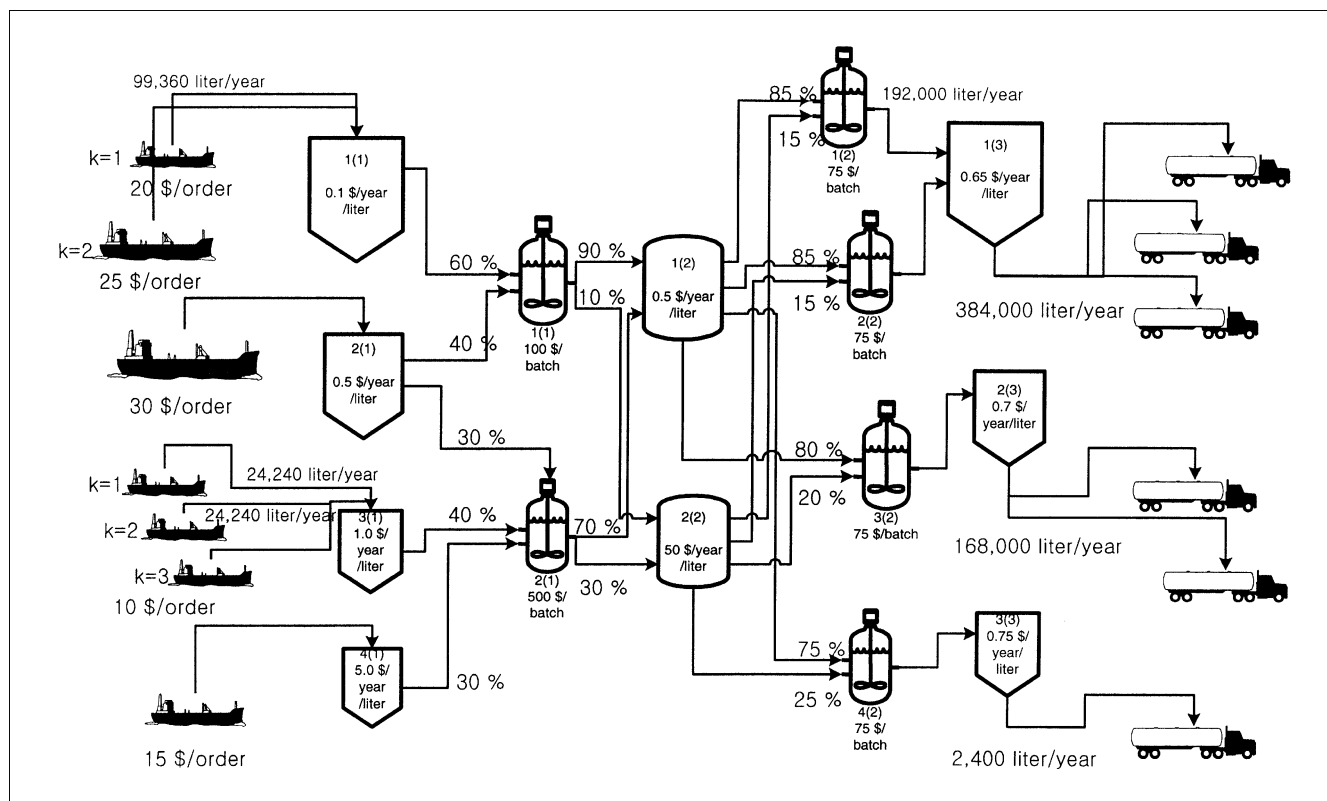


Figure 8. Example plant-input data.

although we can deal with arbitrary periodic demands. All indices are numbered from the top equipment down, as shown in Figure 8. All transportation time fractions are set to zero. We will not consider for convenience capital costs. Raw material 1(1) has two suppliers with order setup costs of \$20 and \$25. The order setup cost for raw material 2(1) is \$30 from a single supplier. The inventory holding costs for raw materials are 0.1, 0.5, 1, and 5 \$/year/L, respectively. The first-stage processes consist of chemical reactions which consume multiple feedstock materials and generate multiple products with different compositions. The compositions are denoted in Figure 8. The setup costs of first stage processes are 100 and 500 \$/Batch. The second-stage processes produce only one product with setup costs 75 \$/Batch. Each product from each process has its dedicated product storage. The inventory holding costs of finished product 1(3), 2(3) and 3(3) are 0.65, 0.7, 0.75 \$/L/year, respectively. The average demand rate for finished products are 384,000, 168,000, and 2,400 L/year, respectively. All demand patterns are constant. The first delivery of the three products will be one year later. The differences between this example and the example treated in our previous work (Yi and Reklaitis, 2000) are in the following: (a) this example has multiple suppliers of raw material 1(1) and 3(1); (b) this example has more than 2 stages; and (c) this example has multiple processes to produce the same product.

According to the design procedure, all average material flow rates through storage units and processes should be calculated. Note that finished product 1(3) has two similar processes 1(2) and 2(2). According to optimality, only one process that has the minimum of  $A_{i(n)}\Psi_{i(n)}$  should be selected,

but, in this example, the average flow rates are assumed to be equally split between two similar processes. The same is true for deciding the average purchase rate of multiple suppliers of raw material 1(1) and 3(1). Then, by using Eqs. 35 and 52, the optimal purchase or batch sizes of all processes are calculated. For example, the optimal lot size of raw material 1(1) is

$$B_1^{1(1)} = \sqrt{\frac{2(20)(99,360)}{0.1}} = 6,304 \text{ L/Batch}$$

The optimal batch size of process 1(1) is

$$B_{1(1)} = \sqrt{\frac{2(100)(372,600)}{(0.1*0.6 + 0.5*0.4 + 0.5*0.9 + 50*0.1)}} = 3,612 \text{ L/Batch}$$

After calculating the optimal batch sizes, optimal storage sizes are calculated by using Eq. 54. For example, the size of intermediate storage 1(2) is

$$V_s^{1(2)} = 0.9*3613 + 0.7*3232 + 0.85*1833 + 0.85*1833 + 0.8*1507 + 0.75*163 = 9958 \text{ liters}$$

Since the first shipment to customers is supposed to take place after one year, the latest startup times of all processes can be calculated by Eqs. 2 and 53 in a backward network

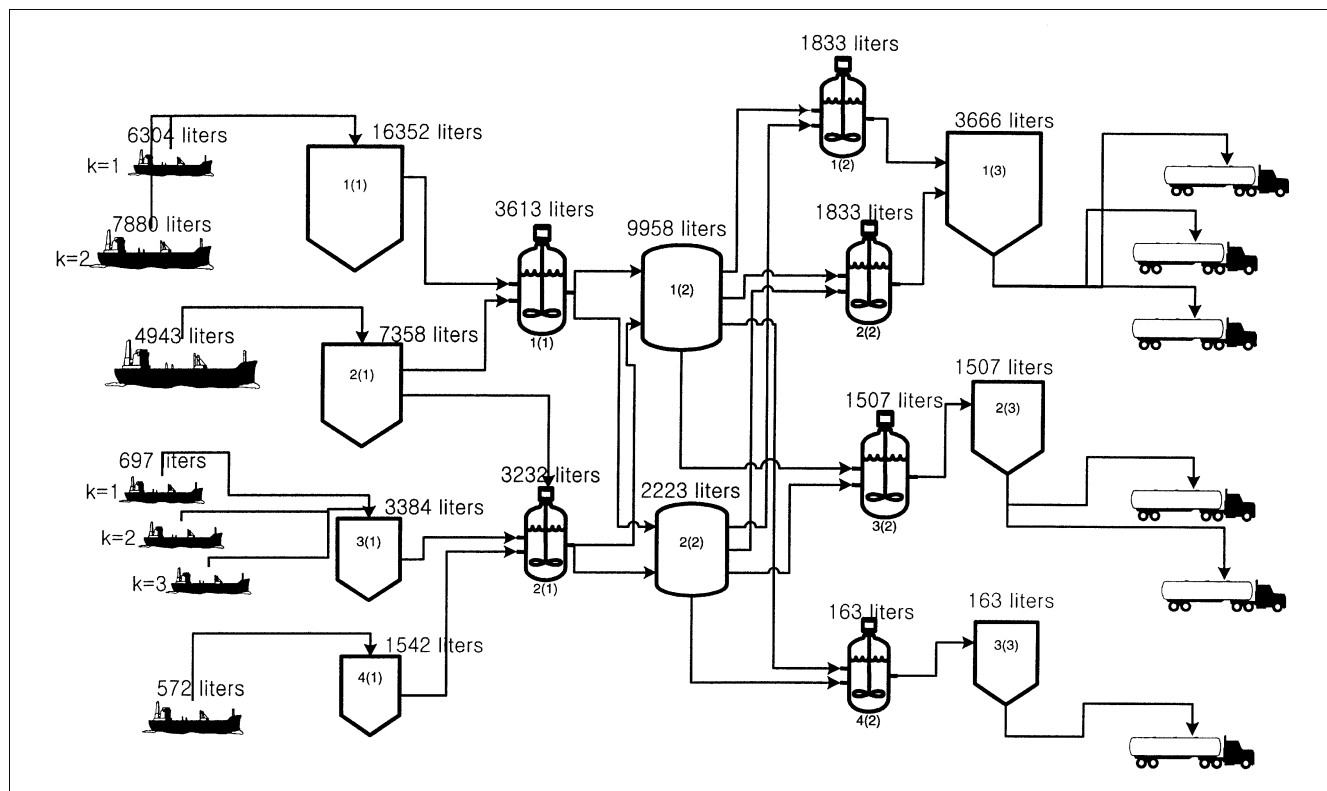


Figure 9. Example plant-calculation results.

direction. Note that these process startup times are operational variables. The optimal plant design is realized not only by optimizing with respect to the design variables, but also by optimizing with respect to the operational variables. The calculated results are summarized in Figure 9.

The constraints for the optimal plant design used in this study were that there is no depletion of storage materials represented by Eqs. 21–23. There can be many other constraints that can be considered in plant design. We will discuss some of them.

(1) The process capacity commonly has maximum and minimum limits. These constraints are easily treated considering that the objective function (Eq. 19) is convex with respect to capacity. If the optimal process capacity obtained by the design procedure in this study is out of range, the nearer extreme value is the optimal solution.

(2) When storage capacity is constrained by a maximum value, an analytic solution may not be possible. Subsequent research will follow on this subject.

(3) How can the procedure developed in this study be applicable to a continuous process? Theoretically, a continuous process does not require a storage unit and the average material flow rate is the capacity itself. However, as many storage units can be seen in a major chemical plant, because most continuous processes operate in a noncontinuous mode. Most continuous processes require a regular shutdown for maintenance, usually one month per year. Some bulk polymer processes such as polyethylene and polypropylene operate in block mode. The block operation means that the processes operate continuously but they keep changing the product

without turning the process off. The noncontinuous operation of such a continuous process can be modeled by using the PSW model with additional timing constraints.

(4) Multiple packaged and/or solid products can be stored in one warehouse. The capacity of warehouse is the sum of the result calculated by Eq. 54 for each product.

(5) If the feedstock composition and/or product yield are variable, the most conservative values should be used for approximation. The exact solution may require large-scale nonlinear programming in this case.

(6) The material transportation between processes and storage units can be a bottleneck in the plant design. In an actual plant, the capacity of a piping network among equipment is mostly insufficient. Several vehicle types are used to deliver the raw materials from long distance suppliers. The vehicle traffic conditions may not allow the assumption of constant transportation time fraction used in this study. This can be addressed by adding virtual processes and storage units with proper parameters.

(7) Although the optimality condition suggests that one should select one supplier among multiple ones and one process among similar processes in the same group, multiple suppliers or multiple similar processes are unavoidable because of many other factors that our objective function does not accommodate. When the lower bounds on the average material flow rates of similar processes in the same group are positive values, the selection guides suggested by Proposition II are still valid with slight modification.

The global minimum point of concave objective function subject to concave polyhedral constraints exists on an ex-

treme point. Therefore, the optimum average material flow rates of similar processes or multiple suppliers take the lower bounds except one process or one supplier.

## Conclusions

This article determines the optimal sizes of batch processes and storage units interconnected in a network structure. These results are useful for the conceptual design of a multiproduct, multistage production and inventory system. The PSW model introduced in our previous work (Yi and Reklaitis, 2000) was used to effectively represent the material flow between the process and storage unit. The objective function for plant design includes minimizing the sum of the process setup costs, inventory holding costs, the capital costs of constructing processes and storage units, and the raw material order setup costs. The constraints of the optimization problem include no depletion of all material inventories in storage units while meeting the finished product demand. The Kuhn-Tucker conditions of optimality were solved analytically under the condition that the number of process groups with a different product yield is equal to the number of products. A simple plant design procedure was proposed based on the analytic solution.

The characteristics of analytic solution derived in this study are as follows: The optimal size of a process in Eq. 52 is determined by the balance between setup and inventory holding cost. The capital cost has the same role of inventory holding cost. The inventory storage units influencing the process size are confined within the storage units directly connected to the process, and the effect of each storage unit is proportional to the average material flow rate between the storage unit and the process. The optimal size of a storage unit in Eq. 54 is the sum of periodic batch sizes coming into or going out from the storage units. When there exist similar multiple processes, only one process should be selected. The optimal solution of the plant design involves not only determining equipment sizes, but also determining the timing of the dispatching operations to meet the finished product delivery, as shown at Eq. 53.

The strength of this study comes from the simplicity of design equations in spite of a general plant structure that can cover a large-scale supply chain. Simple design equations are useful for a diverse situation at the preliminary plant design stage. They will provide a very good initial guess when designers use a sophisticated design algorithm at the detailed design stage. The application of this study is not confined to the plant design. This study will also contribute to the optimal scheduling and operation of the large-scale supply chain, including diagnostic analysis. The optimality and simplicity of the analytical lot sizing solution opens the possibility for designing self-optimizing, real-time scheduling and inventory control systems of large-scale batch-storage network.

## Acknowledgment

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## Notation

$a_k^{j(1)}$  = annualized capital cost of raw material purchasing facility, dollars per unit of item per year

$a_{i(n)}$  = annualized capital cost of unit  $i(n)$ , dollars per unit of item per year  
 $b^{j(n)}$  = annualized capital cost of storage facility, dollars per unit of item per year  
 $A_k^{j(1)}$  = ordering cost of feedstock materials, dollar per order  
 $A_{i(n)}$  = ordering cost of noncontinuous units, dollar per order  
 $B_k^{j(1)}$  = raw material order size, units per lot  
 $B_{i(n)}$  = noncontinuous unit size, units per lot  
 $B_m^{j(N+1)}$  = final product delivery size, units per lot  
 $D_k^{j(1)}$  = average material flow of feedstocks/products, units per year  
 $D_{i(n)}$  = average material flow through noncontinuous units, units per year  
 $f_{i(n)}^{j(n)}$  = feedstock composition of unit  $i(n)$   
 $f_{i(n)}^{j(n+1)}$  = product yield of unit  $i(n)$   
 $H^{j(n)}$  = annual inventory holding costs, dollars per unit of item per year  
 $|kj(1)|$  = number of raw materials  
 $|j(n)|$  = number of intermediate products  
 $|mj(N+1)|$  = number of customers for product  $j(N+1)$   
 $t_m^{j(N+1)}$  = initial delay time of customer demand  
 $t_{i(n)}^{j(n)}$  = initial delay time of feedstock feeding to noncontinuous unit  $i(n)$   
 $t_{i(n)}^{j(n+1)}$  = initial delay time of product discharging from noncontinuous unit  $i(n)$   
 $t_k^{j(1)}$  = initial delay time of raw material purchasing  
 $V_{ub}^{j(n)}$  = upper bound of inventory holdup, units of item  
 $V_{lb}^{j(n)}$  = lower bound of inventory holdup, units of item  
 $V^{j(n)}(t)$  = inventory holdup, units of item  
 $V^{j(n)}(0)$  = initial inventory holdup, units of item  
 $V_s^{j(n)}$  = storage size, units of item  
 $\overline{V}^{j(n)}$  = time averaged inventory holdup, units of item  
 $x_k^{j(1)}$  = transportation time fraction of purchasing raw materials  
 $x_{i(n)}^{j(n)}$  = transportation time fraction of feeding to noncontinuous unit  $i(n)$   
 $x_{i(n)}^{j(n+1)}$  = transportation time fraction of discharging from noncontinuous unit  $i(n)$   
 $x_m^{j(N+1)}$  = transportation time fraction of customer demand  
 $z_p$  = nonnegative variables used in Proposition II  
 $Z$  = a constant used in Proposition II  
 $\alpha_m$  = positive parameters used in Proposition II  
 $\lambda_{lb}^{j(n)}$  = Lagrange multipliers  
 $\lambda_D^{j(n)}$  = Lagrange multipliers  
 $\omega_m^{j(N+1)}$  = cycle time of customer demand, yr  
 $\omega_k^{j(1)}$  = cycle time of raw material purchasing, yr  
 $\omega_{i(n)}$  = cycle time of noncontinuous units, yr  
 $\Psi_{i(n)}$  = defined by Eq. 38

## Subscripts

$i(n)$  = noncontinuous unit index of  $n$ th stage  
 $l(n)$  = similar process group index in  $n$ th stage  
 $k$  = raw material vendors  
 $m$  = finished product customers

## Superscripts

$j(1)$  = raw material index  
 $j(n)$  = intermediate product index of  $n$ th stage  
 $j(N+1)$  = final product index  
 $p$  = used in Proposition II  
 $n$  = stage index based on inventory point

## Special functions

$\text{int}[\cdot]$  = truncation function to make integer  
 $\text{res}[\cdot]$  = positive residual function to be truncated  
 $u(\cdot)$  = unit step function

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## Appendix: Periodic Square Wave Model

Consider the storage connected with only one supply process and one consumption process in Figure 5. The differential material balance around storage  $j(n+1)$  in Figure 5 consists of a simple ordinary differential equation that includes the periodic square wave flow functions. The integration of the material balance equation gives

$$V^{j(n+1)}(t) = V^{j(n+1)}(0) + \int_0^t F_u(\tau) d\tau - \int_0^t F_d(\tau) d\tau \quad (\text{A1})$$

where  $V^{j(n+1)}(t)$  and  $V^{j(n+1)}(0)$  are the current and initial inventory of storage  $j(n+1)$  and  $F_u(t)$  and  $F_d(t)$  are its incoming and outgoing material flows. Each integral can be calculated by directly taking into account the periodic square wave form of the functions  $F_u(t)$  and  $F_d(t)$ . In order to develop the first integral, as shown in Figure A1, for the given time  $t$ , the number of complete cycles are given by  $\text{int}[(t - t_{i(n)}^{(n+1)})/\omega_{i(n)}]$  and the mass corresponding to the completed cycles is  $(f_{i(n)}^{j(n+1)} B_{i(n)} \text{int}[(t - t_{i(n)}^{(n+1)})/\omega_{i(n)}])$ . For the remaining time  $\text{res}[t - t_{i(n)}^{(n+1)}/\omega_{i(n)}]$ , which is less than one cycle in length, there are two cases to consider. If  $\text{res}[(t - t_{i(n)}^{(n+1)})/\omega_{i(n)}]$  is larger than  $x_{i(n)}^{(n+1)}$ , another full cycle has to be added to  $(f_{i(n)}^{j(n+1)} B_{i(n)} \text{int}[(t - t_{i(n)}^{(n+1)})/\omega_{i(n)}])$ . If it is less than  $x_{i(n)}^{(n+1)}$ , the hatched area within the cycle, shown in Figure A1, which is equal to

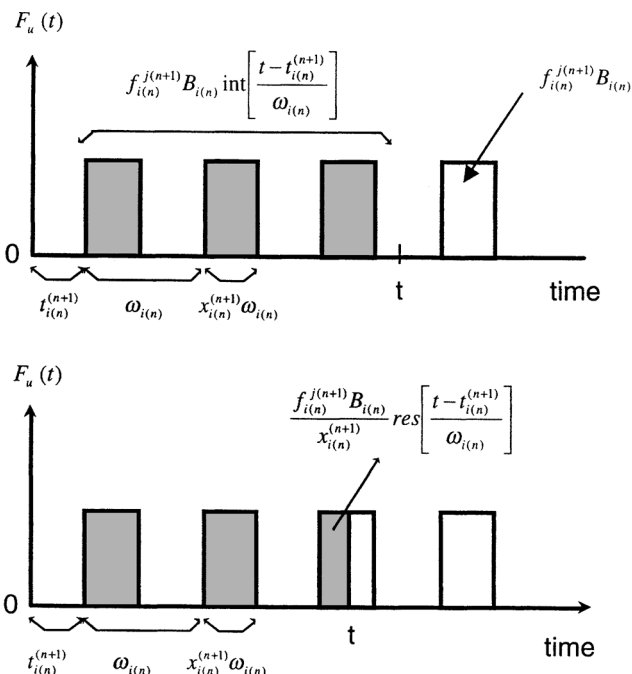


Figure A1. Integration of periodic square wave material flow.

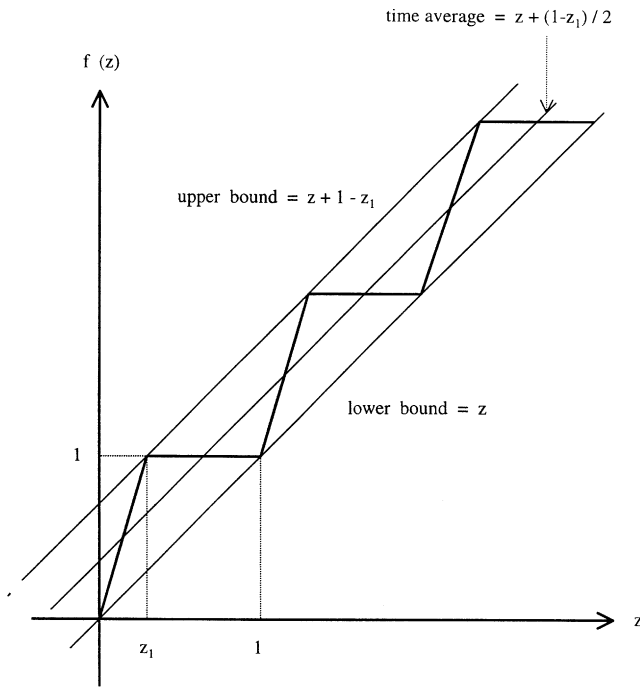
$(f_{i(n)}^{j(n+1)} B_{i(n)} / x_{i(n)}^{(n+1)}) \text{res}[(t - t_{i(n)}^{(n+1)})/\omega_{i(n)}]$ , has to be added. These two cases can be combined into one expression using the  $\min\{\cdot\}$  function.

$$\int_0^t F_u(\tau) d\tau = (f_{i(n)}^{j(n+1)} B_{i(n)}) \times \left[ \text{int} \left( \frac{t - t_{i(n)}^{(n+1)}}{\omega_{i(n)}} \right) + \min \left\{ 1, \frac{1}{x_{i(n)}^{(n+1)}} \text{res} \left( \frac{t - t_{i(n)}^{(n+1)}}{\omega_{i(n)}} \right) \right\} \right] \quad (\text{A2})$$

The second integral of Eq. A1 has the same form. The storage  $j(n+1)$  in the network structure, as shown at Figure 4, is actually connected with  $|i(n)|$  supply processes and  $|i(n+1)|$  consumption processes. Each supply or consumption material flow can be represented in the same as Eq. A2. The complete form of the inventory holdup equation is the sum of these supply and consumption material flows

$$V^{j(n+1)}(t) = V^{j(n+1)}(0) + \sum_{i=1}^{|i(n)|} (f_{i(n)}^{j(n+1)} B_{i(n)}) \left[ \text{int} \left( \frac{t - t_{i(n)}^{(n+1)}}{\omega_{i(n)}} \right) + \min \left\{ 1, \frac{1}{x_{i(n)}^{(n+1)}} \text{res} \left( \frac{t - t_{i(n)}^{(n+1)}}{\omega_{i(n)}} \right) \right\} \right] - \sum_{i=1}^{|i(n+1)|} (f_{i(n+1)}^{j(n+1)} B_{i(n+1)}) \left[ \text{int} \left( \frac{t - t_{i(n+1)}^{(n+1)}}{\omega_{i(n+1)}} \right) + \min \left\{ 1, \frac{1}{x_{i(n+1)}^{(n+1)}} \text{res} \left( \frac{t - t_{i(n+1)}^{(n+1)}}{\omega_{i(n+1)}} \right) \right\} \right] \quad (\text{A3})$$





**Figure A2. Bounds on flow accumulation function.**

Equation A3 corresponds to Eq. 7 in the main text. Equations 6 and 8 in the main text can be obtained as the same way. Equation A3 includes a basic functional group, called the Flow Accumulation Function

$$f(z) = \text{int}[z] + \min\left\{1, \frac{1}{z_1} \text{res}[z]\right\} \quad (\text{A4})$$

The flow accumulation function has the following useful relationships

$$z \leq f(z) \leq z + 1 - z_1 \quad (\text{A5})$$

A linear function  $L(z)$  such that

$$\min_{L(z)} \int_0^\infty |f(z) - L(z)| dt = z + \frac{1 - z_1}{2} \quad (\text{A6})$$

These equations are obvious from Figure A2. The upper/lower bounds and time averaged inventory holdup of Eq. A3 is easily obtained by using Eqs. A5 and A6

$$\begin{aligned} V_{ub}^{j(n+1)} &= V^{j(n+1)}(0) + \sum_{i=1}^{|i(n)|} (1 - x_{i(n)}^{(n+1)}) f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} \\ &- \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(u+1)} \quad (\text{A7}) \end{aligned}$$

$$\begin{aligned} V_{lb}^{j(n+1)} &= V^{j(n+1)}(0) - \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n+1)} \\ &- \sum_{i=1}^{|i(n+1)|} (1 - x_{i(n+1)}^{(n+1)}) f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} \\ &+ \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \quad (\text{A8}) \end{aligned}$$

$$\begin{aligned} \overline{V^{j(n+1)}} &= V^{j(n+1)}(0) + \sum_{i=1}^{|i(n)|} \frac{(1 - x_{i(n)}^{(n+1)})}{2} f_{i(n)}^{j(n+1)} D_{i(n)} \omega_{i(n)} \\ &- \sum_{i=1}^{|i(n)|} f_{i(n)}^{j(n+1)} D_{i(n)} t_{i(n)}^{(n+1)} - \sum_{i=1}^{|i(n+1)|} \frac{(1 - x_{i(n+1)}^{(n+1)})}{2} \\ &\times f_{i(n+1)}^{j(n+1)} D_{i(n+1)} \omega_{i(n+1)} + \sum_{i=1}^{|i(n+1)|} f_{i(n+1)}^{j(n+1)} D_{i(n+1)} t_{i(n+1)}^{(n+1)} \quad (\text{A9}) \end{aligned}$$

Equations A7–A9 correspond to Eqs. 12–14 in the main text. Equations 9–11 and 15–17 can be obtained as the same way.

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