Optimal Design of Batch-Storage Network with Multitasking Semi-continuous Processes

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The periodic square wave (PSW) model was successfully applied to the optimal design of a batch-storage network. The network structure can cover any type of batch production, distribution, and inventory system, including recycle streams. Here we extend the coverage of the PSW model to multitasking semi-continuous processes as well as pure continuous and batch processes. In previous solutions obtained using the PSW model, the feedstock composition and product yield were treated as known constants. This constraint is relaxed in the present work, which treats the feedstock composition and product yield as free variables to be optimized. This modification makes it possible to deal with the pooling problem commonly encountered in oil refinery processes. Despite the greater complexity that arises when the feedstock composition and product yield are free variables, the PSW model still gives analytic lot sizing equations. The ability of the proposed method to determine the optimal plant design is demonstrated through the example of a high density polyethylene (HDPE) plant. Based on the analytical optimality results, we propose a practical process optimality measure that can be used for any kind of process. This measure facilitates direct comparison of the performance of multiple processes, and hence is a useful tool for diagnosing the status of process systems. The result that the cost of a process is proportional to the square root of average flow rate is similar to the well-known six-tenths factor rule in plant design. © 2005 American Institute of Chemical Engineers *AIChE J,* 52: 269–281, 2006
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Introduction

A novel production and inventory analysis method called the periodic square wave (PSW) method has been suggested and used to determine the optimal design of a parallel batch-storage system.[1] Subsequently, the method was extended to handle sequential multistage batch-storage networks,[2] and further modified to handle a non-sequential network structure that can deal with recycle material flows in a plant.[3] The key advantage of the PSW model over existing models lies in its simple analytical sizing and timing equations. This advantageous characteristic was exploited in an analysis of an integrated financial and production system.[4] In the present study, the range of physical plant structures for which the PSW model can be used is enlarged from batch processes to multitasking batch or semi-continuous processes.

Semi-continuous processes are very common in commodity polymer processes, such as HDPE, polypropylene (PP), low

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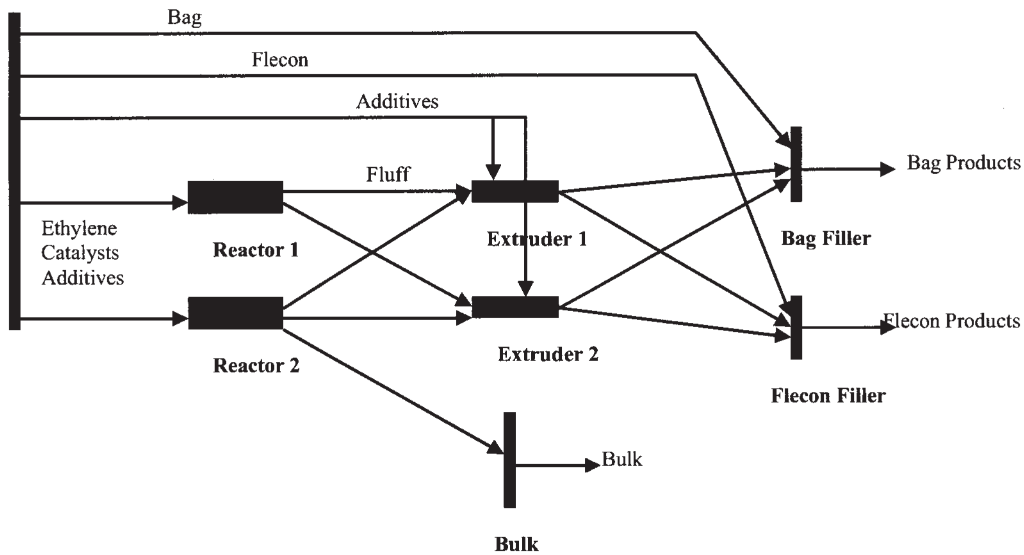

Figure 1. HDPE plant block diagram.

density polyethylene (LDPE), linear low density polyethylene (LLDPE), polyvinyl chloride (PVC), polystyrene (PS), acrylonitrile butadiene styrene (ABS), carbon black (CB), polybutene (PB), and resins. Lubrication base oil processes, solvent processes, and continuous casting in steel-making processes are also operated in the semi-continuous mode. Variable feedstock composition and product yield, which are very popular in oil refinery and petrochemical processes, can also be effectively treated within the proposed model.

Optimal scheduling of semi-continuous processes is an important research subject in process system engineering. Many excellent mixed integer linear programming (MILP) models have been proposed.[5] Recently, a comparison of the continuous-time model has been reported.[6] In the present study, we focus on the theoretical aspects of process optimality for the design and scheduling of semi-continuous processes. We use the PSW model to derive an analytic solution for the optimal lot size or production run length for semi-continuous processes producing multiple products. In the analysis, we consider sequence-dependent change-over costs, inventory holding cost, and capital cost of facilities as objective terms to be minimized. Based on the simple analytic solution derived, we suggest a measure of process design optimality that is applicable to any type of process and an easy near-optimal plant design procedure. Chemical companies commonly possess a range of processes for producing a variety of chemicals. The ability to express the optimality level of each of these distinct processes with the same measure would facilitate decision-making regarding the work sequence of retrofit/revamping design or scheduling/operation optimization. Importantly, it would enable the ranking of processes according to their optimality, making it possible to devote limited resources to fixing the least optimal processes first. In addition to manufacturing processes, the method presented here can be extended to supply chain optimization by including transportation processes among multiple plants and/or distribution centers. This extension can be easily implemented by modeling transportation processes as batch processes without material conversion. In summary, the generalized batch-storage network suggested here can be applied to most kinds of production, inventory, and distribution systems, including batch, semi-continuous, and transportation processes. Based on the results of this study, we suggest an easy optimal design procedure that is suitable for complex systems. For simplicity, we do not discuss the business processes of financial transactions and cash flows treated previously[4]; however, the methods could easily be extended to such processes.

A Motivating Example—HDPE Plant Design

HDPE is a fluff state polymer produced by low pressure suspension, solution, or gas phase polymerization of ethylene. Figure 1 shows a simplified block diagram of the HDPE process. The plant is composed of 2 reactors, 2 extruders, and many silos. It produces 11 grades, each of which has three package types: bag, flecon, or bulk. The bag and flecon products are stored in a warehouse, but the bulk products are shipped directly to the customer. The major raw material, ethylene, is produced by upstream naphtha crackers, and there is no constraint on the supply of raw materials. The reactor is operated in a block mode, and the production rate is almost constant. Some pairs of products should not be produced consecutively because this would introduce sudden property changes. The reactor operates 24 hours a day, 7 days a week, but the packaging operation is conducted during the daytime on weekdays because it is labor intensive operation. In the initial stage of plant design, designers would like to quickly determine a rough estimate of the process and storage capacities required to meet the estimated demand for the finished product. A detailed optimization model, ideally an MILP model,[7] can be used to determine the optimal design solution. However, because detailed information is not available in the early stages of plant design, a rigorous detailed model may be of limited value. In particular, it is common for managerial and strategic decisions to be revised repeatedly during the early stages of plant design as new market information comes to hand. Such revisions can lead to repeated revisions of the subsequent design work. Given this situation, a design method based on a simple

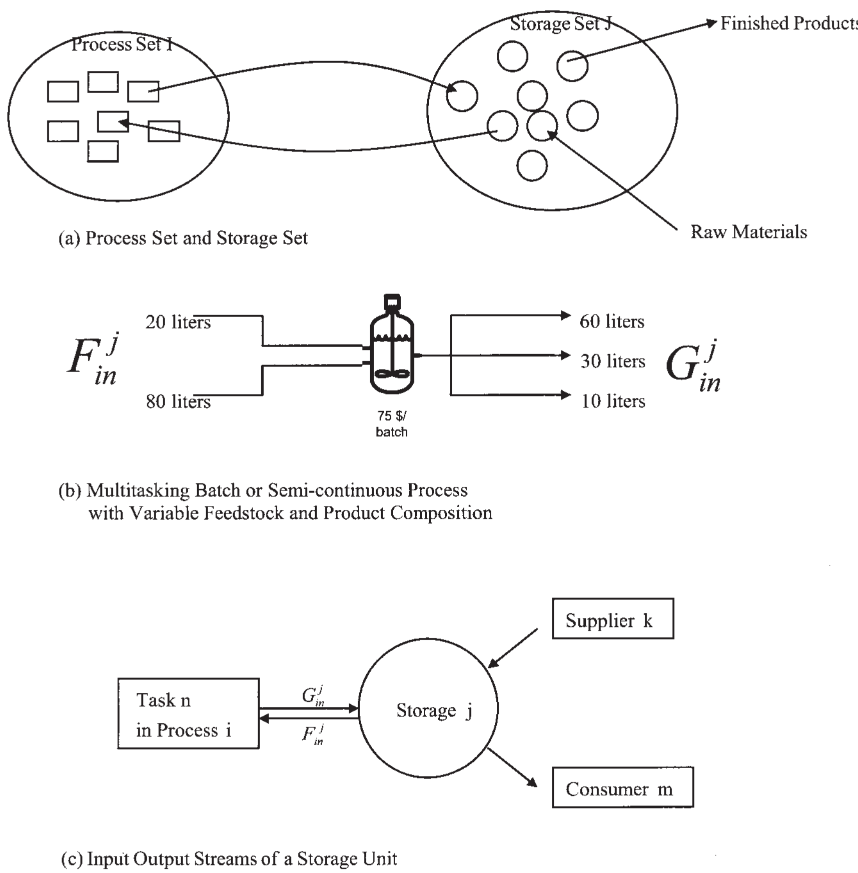

Figure 2. General structure of batch-storage network.

(a) Process set and storage set, (b) Multitasking batch or semi-continuous process with variable feedstock and product composition, (c) Input output streams of a storage unit.

analytic equation is advantageous because it can be used to quickly respond to a diverse range of managerial decisions. In this study, we develop analytical equations for the optimal design of multitasking semi-continuous processes and apply them to the HDPE plant design problem.

The assumptions used in this study are summarized as:

(i) All operations including task sequence are periodical (model).

(ii) No stock-outs are allowed in all storage units (optimization constraint).

(iii) Average flow rates through network are not time-varying (variable definition).

These assumptions can be relaxed in the future studies.

Optimization Model

The definitions and notations used here are mostly the same as the author's previous work.[3] Consider a multitasking batch or semi-continuous process $i \in I$, as shown in Figures 2a and b. This process conducts multiple tasks in sequence, where $n \in N(i)$ is the task index, as shown in Figure 3. Tasks are conducted in the sequence $n = 1, 2, \ldots, |N(i)|$, and this sequence is repeated periodically. If there is only one task in one process, the results of the present study reduce to the author's previous work.[3] The process is fed from feedstock storage units $j \in J$ and produces multiple products. Note that each storage unit stores a single type of material whose material index is also $j \in J$. Each task has different feedstock materials and products. The flow rate of feedstock j to task n in process i is F_{in}^j, and the flow rate of product j from task n in process i is G_{in}^j. Note that feedstock composition and product yield are not constant in this formulation. The material balance around task n in process i gives

$$\sum_{j=1}^{|J|} F_{in}^j = \sum_{j=1}^{|J|} G_{in}^j = \frac{B_{in}}{\omega_{in}} \quad \forall\, i, n \tag{1}$$

where B_{in} and ω_{in} are the batch size and duration, respectively, of task n in process i.

Each process has a common production cycle ω_i and startup time $'t_i$, as shown in Figure 3. The ratio of ω_{in} to ω_i is denoted the cycle time ratio y_{in}, that is, $\omega_{in} \equiv y_{in}\omega_i$ where $\sum_{n=1}^{|N|} y_{in} =$

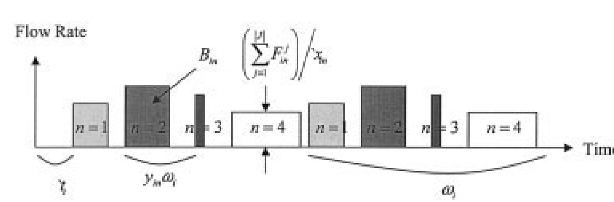

Figure 3. Multitasking batch process.

1 and $0 \leq y_{in} \leq 1$. The cycle time ratio y_{in} will be considered as a parameter in the later development of Kuhn-Tucker conditions of optimality. In fact, y_{in} depends on the task sequence and could be made a variable by including the minimization of the sequence dependent cost into the optimization scope. The feeding startup time of task n in process i is defined as ${}^{\backprime}t_{in}$, and the discharging startup time of task n in process i is defined as t'_{in}. Under these definitions, the following timing relationships hold

$$t'_{in} = {}^{\backprime}t_{in} + \Delta t_{in} \quad \forall\, i, n \tag{2}$$

$${}^{\backprime}t_{in} = {}^{\backprime}t_{i} + \omega_i \sum_{n'=1}^{n-1} y_{in'} \quad \forall\, i, n \tag{3}$$

where Δt_{in} is the difference between the feeding and discharging startup times of task n in process i. Note that this startup time difference is the sum of the feeding time and processing time and can be expressed as an arbitrary function of the cycle times or other design variables. For example, Δt_{in} was set to $\omega_{in}(1 - x'_{in})$ in the author's previous work[3] where (${}^{\backprime}x_{in}$ and) x'_{in} are parameters defined as (feeding and) discharging storage operation time fractions that are less than or equal to 1. This expression is reasonable for production processes but is not valid for transportation processes in a supply chain. For transportation processes, it is reasonable to set Δt_{in} to a constant value. The overall material balance around storage unit j gives

$$\sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} G^j_{in} y_{in} + \sum_{k=1}^{|K(j)|} D^j_k = \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} F^j_{in} y_{in} + \sum_{m=1}^{|M(j)|} D^j_m \quad \forall\, j \tag{4}$$

where D^j_k is the average flow rate of material j purchased from supplier $k \in K(j)$ and D^j_m is the average flow rate of the demand for material j by customer $m \in M(j)$. The constraint of the pooling problem has the following form

$$\sum_{j=1}^{|J(i,n)|} \theta^j F^j_{in} = \theta \sum_{j'=1}^{|J'(i,n)|} G^{j'}_{in}, \quad J(i, n) \cap J'(i, n) = \varnothing \quad \forall\, i, n \tag{5}$$

where θ^j is the physical property of feedstock material $j \in J(i, n)$ and θ is the physical property of product $j' \in J'(i, n)$.

The incoming material flows of purchased feedstock materials are defined by the average flow rate D^j_k, cycle time ω^j_k, startup time t^j_k, and storage operation time fraction x^j_k, where the batch size $B^j_k = D^j_k \omega^j_k$. The average flow rate D^j_m, batch size B^j_m, cycle time ω^j_m, startup time t^j_m, and storage operation time fraction x^j_m of the finished product demands are known constants where $B^j_m = D^j_m \omega^j_m$.

Multiple tasks sharing a common production period in process i cannot be directly represented by the PSW flow model. The flow of multiple tasks can be decomposed into multiple flows of a periodic single task, as shown in Figure 4. Then, by using the machinery of the PSW model with respect to the flow of each task and summing the results of the single task representations, we can obtain the representation for multiple tasks.

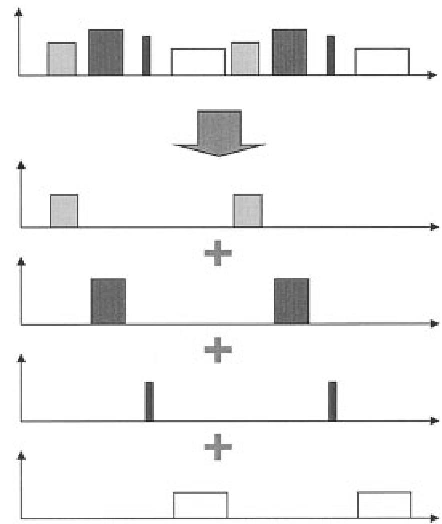

Figure 4. Decomposition of multiple tasks into multiple flows of single task.

Consequently, the inventory holdup $V^j(t)$ of storage unit j is represented by the PSW model in the same way as in the author's previous work.[3] A storage unit is connected to incoming flows from suppliers and processes, and outgoing flows to consumers and processes as shown in Figure 2c. The integration of each PSW flow from initial time to current time equals the batch size multiplied by the integer part of the time interval over cycle time, plus an additional term less than or equal to the batch size. That is, the integration of each flow has the form of $B[\mathrm{int}[(t - t')/\omega] + \min\{1, (1/x)res[(t - t')/\omega]\}]$ where B = batch size, t = time, t′ = startup time, ω = cycle time, and x = storage operation time fraction, derived from the shape of the periodic square wave.[1] The inventory holdup function $V^j(t)$ for storage unit j can be calculated by adding all incoming flows and subtracting all outgoing flows from the initial inventory

$$\begin{aligned} V^j(t) = V^j(0) &+ \sum_{k=1}^{|K(j)|} B^j_k \left[\mathrm{int}\left[\frac{t - t^j_k}{\omega^j_k}\right] + \min\left\{1, \frac{1}{x^j_k}\, res\left[\frac{t - t^j_k}{\omega^j_k}\right]\right\}\right] \\ &+ \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (G^j_{in}\omega_{in}) \left[\mathrm{int}\left[\frac{t - t'_{in}}{\omega_i}\right] + \min\left\{1, \frac{1}{x'_{in} y_{in}}\, res\left[\frac{t - t'_{in}}{\omega_i}\right]\right\}\right] \\ &- \sum_{m=1}^{|M(j)|} B^j_m \left[\mathrm{int}\left[\frac{t - t^j_m}{\omega^j_m}\right] + \min\left\{1, \frac{1}{x^j_m}\, res\left[\frac{t - t^j_m}{\omega^j_m}\right]\right\}\right] \\ &- \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (F^j_{in}\omega_{in}) \left[\mathrm{int}\left[\frac{t - {}^{\backprime}t_{in}}{\omega_i}\right] + \min\left\{1, \frac{1}{{}^{\backprime}x_{in} y_{in}}\, res\left[\frac{t - {}^{\backprime}t_{in}}{\omega_i}\right]\right\}\right] \quad \forall\, j \end{aligned} \tag{6}$$

where $V^j(0)$ is the initial inventory holdup. Each term of Eq. 6 has a basic functional form $f(z) = \mathrm{int}[z] + \min\{1, (res[z]/z_1)\}$, which is called the flow accumulation function. This function has lower bound z, upper bound $z + 1 - z_1$, and average z + 0.5(1 − z_1), which are obvious from the graphical representation of $f(z)$.[2] The upper bound of the inventory holdup, the lower bound of the inventory holdup, and the average inventory holdup can be calculated by using these properties of the flow accumulation function. The upper bound of inventory will be used to compute the capital cost of the storage unit. The lower bound of inventory will be used for the optimization constraint. The average inventory level will be used to compute inventory holding cost. The upper and lower bounds of the inventory holdup, $\overline{\overline{V}}^j$ and $\underline{\underline{V}}^j$, respectively, are

$$\overline{\overline{V}}^j = V^j(0) + \sum_{k=1}^{|K(j)|}(1-x_k^j)D_k^j\omega_k^j - \sum_{k=1}^{|K(j)|}D_k^j t_k^j + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} \times (1-x'_{in}y_{in})G_{in}^j\omega_{in} - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} G_{in}^j y_{in} t'_{in} + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} F_{in}^j y_{in}\,{}^{\backprime}t_{in} + \sum_{m=1}^{|M(j)|} D_m^j t_m^j \qquad \forall j \qquad (7)$$

$$\underline{\underline{V}}^j = V^j(0) - \sum_{k=1}^{|K(j)|}D_k^j t_k^j - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} G_{in}^j y_{in} t'_{in} - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} \times (1-{}^{\backprime}x_{in}y_{in})F_{in}^j\omega_{in} + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} F_{in}^j y_{in}\,{}^{\backprime}t_{in} - \sum_{m=1}^{|M(j)|} \times (1-x_m^{in})D_m^j\omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j \qquad \forall j \qquad (8)$$

The average level of the inventory holdup $\overline{V^j}$ is

$$\bar{V}^j = V^j(0) + \sum_{k=1}^{|K(j)|}\frac{(1-x_k^j)}{2}D_k^j\omega_k^j - \sum_{k=1}^{|K(j)|}D_k^j t_k^j + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}\frac{(1-x'_{in}y_{in})}{2}G_{in}^j\omega_{in} - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} G_{in}^j y_{in} t'_{in} - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}\frac{(1-{}^{\backprime}x_{in}y_{in})}{2}F_{in}^j\omega_{in} + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} F_{in}^j y_{in}\,{}^{\backprime}t_{in} - \sum_{m=1}^{|M(j)|}\frac{(1-x_m^j)}{2}D_m^j\omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j \qquad \forall j \qquad (9)$$

The purchasing setup cost of raw material j is denoted by A_k^j \$/order, and the setup (change-over or grade transition) cost of task n of process i is denoted by A_{in} \$/batch. The annual inventory holding cost of storage j is denoted by H^j \$/L/year. The objective function of design optimization is minimizing the total cost, which is composed of purchase setup costs, process setup costs, and inventory holding costs of materials. The capital costs of tasks and storage units are included, as well as the costs related with the average flow rates of purchasing and/or processing flows, which are called material prices

$$TC = \sum_{j=1}^{|J|}\sum_{k=1}^{|K(j)|}\left[\frac{A_k^j}{\omega_k^j} + a_k^j B_k^j + P_k^j D_k^j\right] + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}\left[\frac{A_{in}}{\omega_i} + a_{in}B_{in} + \sum_{j=1}^{|J|} P_{in}^j(F_{in}^j - G_{in}^j)\right] + \sum_{j=1}^{|J|}\left[H^j\overline{V^j} + b^j\overline{\overline{V^j}}\right] \qquad (10)$$

where a_k^j, α_{in}, and b^j are the annualized capital costs of purchasing batch, task processing batch, and storage units; and P_k^j and P_{in}^j are the material prices of the corresponding flows. The lower bound of the inventory holdup (Eq. 8) should be greater than or equal to zero, that is, $\underline{\underline{V}}^j \geq 0$. This constitutes the constraints of the optimization

$$V^j(0) - \sum_{k=1}^{|K(j)|}D_k^j t_k^j - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} G_{in}^j y_{in}\left({}^{\backprime}t_i + \omega_i\sum_{n'=1}^{n-1} y_{in'} + \Delta t_{in}\right) - \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}(1-{}^{\backprime}x_{in}y_{in})F_{in}^j\omega_{in} + \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|} F_{in}^j y_{in}\left({}^{\backprime}t_i + \omega_i\sum_{n'=1}^{n-1} y_{in'}\right) - \sum_{m=1}^{|M(j)|}(1-x_m^{in})D_m^j\omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j \geq 0 \qquad \forall j \qquad (11)$$

Without loss of generality, the storage size will be determined by the upper bound of the inventory holdup $\overline{\overline{V}}^j$. Thus, Eq. 7 is the expression for the storage capacity. The independent variables are selected to be the cycle times (ω_k^j and ω_i), start-up times (t_k^j and ${}^{\backprime}t_i$), average flow rates (D_k^j, F_{in}^j, and G_{in}^j) and cycle time ratios (y_{in}). Note that the start-up times t'_{in} and ${}^{\backprime}t_{in}$ are converted into ${}^{\backprime}t_i$ by using Eqs. 2 and 3.

Solution of Kuhn-Tucker Conditions

The objective function Eq. 10 is convex and the constraints are linear with respect to ω_k^j, ω_i, t_k^j, and ${}^{\backprime}t_i$ if D_k^j, F_{in}^j, G_{in}^j, and y_{in} are considered as parameters. However, the convexity with respect to D_k^j, F_{in}^j, G_{in}^j, and y_{in} is not clear. First, we obtain the solution for Kuhn-Tucker conditions with respect to ω_k^j, ω_i, t_k^j and ${}^{\backprime}t_i$ when D_k^j, F_{in}^j, G_{in}^j, and y_{in} are considered as parameters, after which we will further solve the problem with respect to D_k^j, F_{in}^j, G_{in}^j, and y_{in}. 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.[3] In other words, the Kuhn-Tucker conditions of the first problem produce an explicit analytical solution and the original problem can be reduced to the second problem by eliminating the design variables of the first problem. The first problem of the two-level problem has a convex objective with linear inequality constraints, and the second problem has a non-convex objective with nonlinear equality constraints. The two-level parametric approach leads to a global optimum provided the second problem converges to its global optimum point. The solution of the Kuhn-Tucker conditions of the first problem (see Appendix A for derivation) is as follows

$$^{*}\omega_k^j = \sqrt{\frac{A_k^j}{D_k^j \Psi_k^j}} \tag{12}$$

$$^{*}\omega_i = \sqrt{\frac{\sum_{n=1}^{|N(i)|} A_{in}}{\Psi_i(F_{in}^j, G_{in}^j, y_{in})}} \tag{13}$$

where Ψ_k^j and Ψ_i are aggregated cost terms defined as

$$\Psi_k^j = \left(\frac{H^j}{2} + b^j\right)(1 - x_k^j) + a_k^j \tag{14}$$

$$\Psi_i(F_{in}^j, G_{in}^j, y_{in}) = \sum_{j=1}^{|J|} \sum_{n=1}^{|N(i)|} [a_{in} y_{in} F_{in}^j + (0.5H^j + b^j) \times \{F_{in}^j(1 - {}^{\backprime}x_{in} y_{in}) y_{in} + G_{in}^j(1 - x'_{in} y_{in}) y_{in}\}] \tag{15}$$

Eqs. 14 and 15 can be further improved by including financial cost factors, such as bank interest and material prices.[4] Eq. 13 is identical to the solution of the economic lot scheduling problem (ELSP)[8] if Ψ_i includes only product storage parameters with $x'_{in} = 1$, $b^j = 0$, $G_{in}^j = D_i g_{in}^j$, $g_{ij}^j = 1$, and $g_{in}^j = 0$ for $n \neq j$.

Inspection of Eq. 13 reveals that the optimum point occurs when the sum of setup (or change-over) costs equals the sum of all the other costs (e.g., inventory holding cost and capital cost of facilities), that is, $[(\sum_{n=1}^{|N(i)|} A_{in}/(^{*}\omega_i)] = \Psi_i(F_{in}^j, G_{in}^j, y_{in})(^{*}\omega_i)$ $(\equiv \sqrt{\Psi_i(F_{in}^j, G_{in}^j, y_{in}) \sum_{n=1}^{|N(i)|} A_{in}})$. The degree of deviation from this equality can be a measure of non-optimality. We suggest the following relative optimality gap of process design that can be used when the process does not have cost factors proportional to average material flow rates (price terms)

Relative Optimality Gap of Process i, Type 1

$$= \frac{\left|\frac{\sum_{n=1}^{|N(i)|} A_{in}}{\omega_i} - \Psi_i(F_{in}^j, G_{in}^j, y_{in})\omega_i\right|}{2\sqrt{\Psi_i(^{*}F_{in}^j, {}^{*}G_{in}^j, {}^{*}y_{in}) \sum_{n=1}^{|N(i)|} A_{in}}} \tag{16}$$

An alternative definition of the optimality measure that has a different scale and can be used when the process has cost factors proportional to average material flow rates (price terms) is as follows

$$\text{Relative Optimality Gap of Process } i\text{, Type 2} = \left| \frac{\frac{\sum_{n=1}^{|N(i)|} A_{in}}{\omega_i} + \Psi_i(F_{in}^j, G_{in}^j, y_{in})\omega_i + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \sum_{j=1}^{|J|} P_{in}^j (F_{in}^j - G_{in}^j)}{2\sqrt{\Psi_i(^{*}F_{in}^j, {}^{*}G_{in}^j, {}^{*}y_{in}) \sum_{n=1}^{|N(i)|} A_{in}} + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \sum_{j=1}^{|J|} P_{in}^j (^{*}F_{in}^j - {}^{*}G_{in}^j)} - 1 \right| \tag{17}$$

where the left upper star denotes an optimized value. The denominator of Eqs. 16 and 17 is the sum of all the optimal costs relevant to process i. Eqs. 16 and 17 provide dimensionless quantities that can be used to compare the level of design or scheduling optimality of different processes.

The optimality cannot be determined from lot sizing equations alone. The startup times must satisfy the following linear system at the optimum from Eq. A8

$$\sum_{k=1}^{|K(j)|} D_k^j t_k^j + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (G_{in}^j - F_{in}^j) y_{in} {}^{\backprime}t_i = V^j(0) - \sum_{m=1}^{|M(j)|} (1 - x_m^j) D_m^j \omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \left(\sum_{n'=1}^{n-1} y_{in'}\right)(F_{in}^j - G_{in}^j) y_{in} \omega_i - \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \Delta t_{in} G_{in}^j y_{in} - \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (1 - {}^{\backprime}x_{in} y_{in}) F_{in}^j y_{in} \omega_i \quad \forall j \tag{18}$$

The most cost-effective way to satisfy the equality is to adjust the startup times t_k^j and ${}^{\backprime}t_i$. When the equality cannot be satisfied by varying the design variables within their feasible ranges, the customer demand shipping startup time t_m^j may be delayed. This delay creates an additional cost, called the backlogging or lost sales cost. Estimating this cost is very subjective and nontrivial because it is determined in part by sociological customer behavior. Eq. 18 indicates various other parameters that can be adjusted to satisfy the equality. For example, building a large safety inventory stock, $V^j(0)$, can avoid material deficiencies. Alternatively, if the customer agrees, the product can be purchased from a third party and delivered to the customer. The most cost effective approach is difficult to determine because of uncertain cost parameters related to customer behavior. It is beneficial to consider Eq. 18 at the early stages of plant design so as to ensure that the plant operations are immune from such cost uncertainties. The corresponding optimal objective function is

$$^{*}TC(D_k^j, F_{in}^j, G_{in}^j, y_{in}) = 2 \sum_{j=1}^{|J|} \sum_{k=1}^{|K(j)|} (\sqrt{A_k^j \Psi_k^j D_k^j} + P_k^j D_k^j) + 2 \sum_{i=1}^{|I|} \sqrt{\Psi_i(F_{in}^j, G_{in}^j, y_{in}) \sum_{n=1}^{|N(i)|} A_{in}} + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \sum_{j=1}^{|J|} P_{in}^j (F_{in}^j - G_{in}^j) + \sum_{j=1}^{|J|} \left(\frac{H^j}{2} + b^j\right) \sum_{m=1}^{|M(j)|} D_m^j \omega_m^j (1 - x_m^j) \tag{19}$$

Table 1. The Solution of Kuhn-Tucker Conditions

Design Variables	Non-Negative Variables: D^j_k, D_i, y_{in}, Binary Variables: g^j_{in} and $Z^{jj'}_{in}$
Objective function	$*TC(D^j_k, D_i y_{in}) = 2\sum_{j=1}^{\lvert J\rvert}\sum_{k=1}^{\lvert K(j)\rvert}\sqrt{A^j_k\Psi^j_k D^j_k} + 2\sum_{i=1}^{\lvert I\rvert}\sqrt{\Psi_i(y_{in})D_i\sum_{n=1}^{\lvert N(i)\rvert}A_{in}} + \sum_{j=1}^{\lvert J\rvert}(0.5H^j + b^j)\sum_{m=1}^{\lvert M(j)\rvert}D^j_m\omega^j_m(1 - x^j_m)$
Constraints	$\sum_{i=1}^{\lvert I\rvert}\sum_{n=1}^{\lvert N(i)\rvert}g^j_{in}D_i y_{in} + \sum_{k=1}^{\lvert K(j)\rvert}D^j_k = \sum_{i=1}^{\lvert I\rvert}\sum_{n=1}^{\lvert N(i)\rvert}f^j_{in}D_i y_{in} + \sum_{m=1}^{\lvert M(j)\rvert}D^j_m, \sum_{n=1}^{\lvert N(i)\rvert}y_{in} = 1,$ $A_{in} = \sum_{j=1}^{\lvert J\rvert}\sum_{j'=1}^{\lvert J\rvert}A^{jj'}Z^{jj'}_{in}, \sum_{j=1}^{\lvert J\rvert}Z^{jj'}_{in} = g^{j'}_{i(n+1)}, \sum_{j'=1}^{\lvert J\rvert}Z^{jj'}_{in} = g^j_{in}, \sum_{j=1}^{\lvert J\rvert}g^j_{in} = 1, f^j_{in} = \sum_{j'=1}^{\lvert J\rvert}\phi^{jj'}g^{j'}_{in},$ $\Psi_i(y_{in}) = \sum_{j=1}^{\lvert J\rvert}\sum_{n=1}^{\lvert N(i)\rvert}[a_{in}y_{in} + (0.5H^j + b^j)\{f^j_{in}y_{in}(1 - y_{in}) + g^j_{in}y_{in}(1 - y_{in})\}]$
Cycle times	$\omega^j_k = \sqrt{\frac{A^j_k}{D^j_k\Psi^j_k}}, \omega_i = \sqrt{\frac{\sum_{n=1}^{\lvert N(i)\rvert}A_{in}}{D_i\Psi_i(y_{in})}}$
Start-Up times	$\sum_{k=1}^{\lvert K(j)\rvert}D^j_k t^j_k + \sum_{i=1}^{\lvert I\rvert}\sum_{n=1}^{\lvert N(i)\rvert}(g^j_{in} - f^j_{in})y_{in}D_i {}^{\backprime}t_i$ $= V^j(0) - \sum_{m=1}^{\lvert M(j)\rvert}(1 - x^j_m)D^j_m\omega^j_m + \sum_{m=1}^{\lvert M(j)\rvert}D^j_m t^j_m + \sum_{i=1}^{\lvert I\rvert}\sum_{n=1}^{\lvert N(i)\rvert}\left(\sum_{n'=1}^{n-1}y_{in'}\right)y_{in}(f^j_{in} - g^j_{in})D_i\omega_i$ $- \sum_{i=1}^{\lvert I\rvert}\sum_{n=1}^{\lvert N(i)\rvert}\Delta t_{in}g^j_{in}y_{in}D_i - \sum_{i=1}^{\lvert I\rvert}\sum_{n=1}^{\lvert N(i)\rvert}(1 - y_{in})y_{in}f^j_{in}D_i\omega_i$

Note that the cost terms are separable with respect to each process i. The fact that the cost of a process i is proportional to the square root of average flow rate is similar to the well-known six-tenths factor rule in plant design.[9]

The optimal size of storage units is calculated using the expression for the upper bound of the inventory holdup, Eq. 7, and Eq. 18

$$* \bar{\bar{V}}^j = \sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}[(1 - {}^{\backprime}x_{in}y_{in})F^j_{in}y_{in} + (1 - x'_{in}y_{in})G^j_{in}y_{in}]\omega_i + \sum_{k=1}^{|K(j)|}(1 - x^j_k)D^j_k\omega^j_k + \sum_{m=1}^{|M(j)|}(1 - x^j_m)D^j_m\omega^j_m \quad (20)$$

Second-Level Optimization Problem

The objective function in Eq. 19 should be further minimized with respect to D^j_k, F^j_{in}, G^j_{in}, and y_{in} under the constraints of Eqs. 4 and 5. This second level optimization problem for block operation mode is summarized in Table 1. Semi-continuous processes usually operate in block operation mode. Block operation changes the operating mode or product without turning the processing off and on, as shown in Figure 5. Block operation can be viewed as a special case of multitasking batch processing. If ${}^{\backprime}x_{in} = x'_{in} = 1$, $F^j_{in} = f^j_{in}D_i$, $G^j_{in} = g^j_{in}D_i$, and $\alpha_{in} = \alpha_i$ where f^j_{in} is the feedstock composition (parameter), g^j_{in} is the product yield (parameter), and D_i is the average flow rate (variable), then the multitasking batch processing in Figure 3 changes into the block operation of a semi-continuous process, as shown in Figure 5. Usually, a task produces a single product (i.e., $g^j_{in} = 1$) if the n-th task in process i produces product j, and $g^j_{in} = 0$ otherwise. Thus, when production sequences are considered as variables, g^j_{in} should be a binary variable. In order to consider product change-over cost, another newly defined binary variable is required: $Z^{jj'}_{in} = 1$ if the n-th task in process i produces product j and the (n+1)-th task produces product j', and $Z^{jj'}_{in} = 0$ otherwise. Then, the following additional constraint equations are required[10]

$$A_{in} = \sum_{j=1}^{|J|}\sum_{j'=1}^{|J|}A^{jj'}Z^{jj'}_{in}, \quad \sum_{j=1}^{|J|}Z^{jj'}_{in} = g^{j'}_{i(n+1)},$$

$$\sum_{j'=1}^{|J|}Z^{jj'}_{in} = g^j_{in}, \quad \sum_{j=1}^{|J|}g^j_{in} = 1, \quad f^j_{in} = \sum_{j'=1}^{|J|}\phi^{jj'}g^{j'}_{in} \quad (21)$$

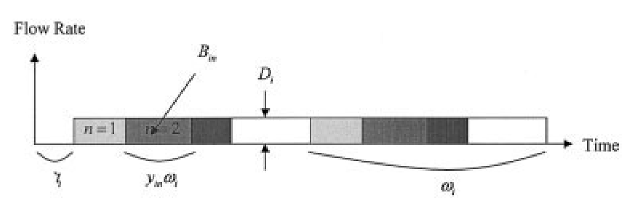

Figure 5. Block operation of semi-continuous process.

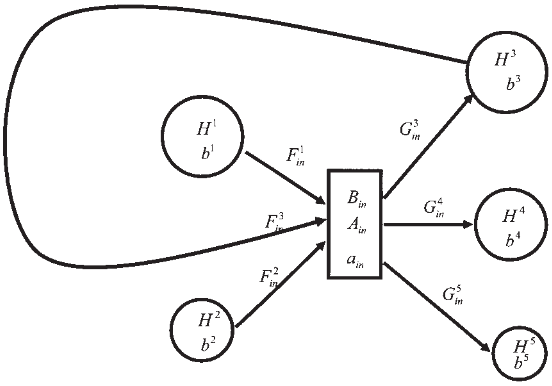

Figure 6. Optimal size of multitasking batch process connected by storage units.

where $A^{jj'}$ is the product change-over (grade transition) cost for changing from product j to product j', and $\phi^{jj'}$ is the composition of feedstock j required to produce product j'.

The second level optimization model for determining the optimal values of the average flow rates through the network, summarized in Table 1, is thus a non-convex mixed integer nonlinear programming (MINLP) problem. It is extremely difficult to find the global optimum for such systems. However, the problem can be simplified somewhat by making the substitution $D_{in} \equiv D_i y_{in}$. The problem can be completely linearized by setting $y_{in} \equiv \sum_{l=0}^{L} (l/L) Y^l_{in}$, $\sum_{l=0}^{L} Y^l_{in} = 1$, where Y^l_{in} is a binary variable, and hence the global optimum of the problem can be obtained. However, this linearization transformation generates a huge number of variables and constraints, including a new binary variable with 7 indices, $\Omega^{jlj'j''}_{inn'} \equiv g^j_{in} Y^l_{in} Z^{j'j''}_{in'}$. In fact, the transformed large-scale MILP problem can only be solved on a high performance computer with a huge memory. In order for the problem to be numerically tractable, the production sequence and either D_i or y_{in} should be determined beforehand, which transforms the problem into separable concave objective minimization.[4] This requirement significantly restricts the applicability of the method; however, there are many real cases that satisfy the above conditions. For example, the LDPE process has only one fixed production sequence following the trend of increasing and decreasing melting index. In addition, technical considerations limit the number of possible production sequences in the PP, LLDPE, PB, and resins processes and, hence, the global optimum for these processes can be easily found by enumerating all the feasible sequences. The scheduling problem has already fixed D_i for most semi-continuous processes. In addition, by invoking the reasoning outlined below, the computational burden of determining the design variables can be reduced to an acceptable level.

Consideration of the second term of Eq. 19 gives further insight into how to solve the problem without severe computation. Suppose we select the production sequence that has the minimum total setup or change-over cost and $\min_n A_{in} > (1/2)\max_{n'} A_{in'}$. Then, splitting production tasks increases the term $[\sum_{n'=1}^{|N(i)|} A_{in'}]$. Suppose task n in process i is split into two tasks, that is, $y_{in} = y^1_{in} + y^2_{in}$. Then, $y_{in}(1 - y_{in}) = (y^1_{in} + y^2_{in})(1 - y^1_{in} - y^2_{in}) < y^1_{in}(1 - y^1_{in}) + y^2_{in}(1 - y^2_{in})$. In general, splitting a task for the same product increases the term Ψ_i. This observation indicates that it is optimal to allocate all different products to the tasks in a common cycle. Eq. 19 is a concave function. Semi-continuous processes usually have multiple processes in parallel, and the total production $\sum_{i=1}^{|I|} D_i$ = total demand = constant. Considering the sluggish nature of the square root function with respect to the increase of its argument, increasing the number of processes $|I|$ for the same total product demand would increase the value of the second term in Eq. 19 and, thus, the total cost. Therefore, the one-process solution is highly likely to be a global optimum, and multiple processes in a plant should be considered as a single super-process. This means that, where possible, production tasks should be allocated so as not to share multiple processes. However, the single super-process solution may not be a global optimum if a significant cost discount is obtained by constructing multiple processes of equal size, as is typically the case in the real world. Note also that the change-over cost, $A^{jj'}$, is a function of the process capacity (D_i). This can make the total cost become a monotonically increasing convex function with respect to D_i, which may make multiple processes more cost effective than a single process. Based on the analytical solution and subsequent analysis, we suggest the following optimal design and operation guidelines:

(i) Reduce the number of processes. Maximize the capacity of one selected process among multiple processes.

(ii) Multiple semi-continuous processes in a plant should be considered as a single super-process.

(iii) Allocate different products to the tasks within one common cycle or try to minimize the number of change-overs (or total change-over cost) within a common cycle.

(iv) Do not share processes or minimize process sharing for the same product.

(v) Use Eq. 13 for lot sizing after determining the production sequence. Determine lot size so that the sum of the fixed charge cost is equal to the sum of the variable costs.

(vi) Use Eq. 20 for storage unit sizes. Optimal storage capacity is the sum of all incoming and outgoing periodic batch sizes with negligible storage operation time.

(vii) Devise a production schedule that minimizes the deviations of Eq. 18. Introduce weighting factors among the deviations of Eq. 18 that are equivalent to the so-called costs of backlogging or lost sales.

Note that the above guidelines are valid when minimum/maximum production run length, maximum inventory, and quantity discounts in construction costs are not considered.

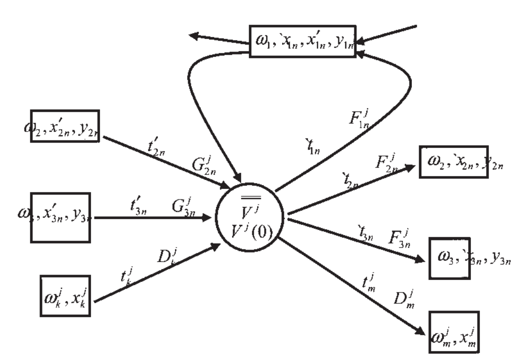

Figure 7. Optimal size of storage unit connected by multiple supply and consumption processes.

Table 2. Grade Transition Costs of HDPE Plant ($/batch)

	F5502	F607LD	F6060P	F50100	TR158	TR570	TR144	TR130	TR147	F5811	HX100
F5502	0	2,040	3,570	4,080	5,610	6,120	4,080	4,590	4,080	4,590	8,160
F607LD	2,889	0	2,408	4,815	4,334	6,741	5,297	5,297	4,815	3,371	9,630
F6060P	2,895	2,413	0	4,825	4,825	6,755	5,308	5,790	4,825	2,895	9,650
F50100	3,206	5,954	6,870	0	3,206	4,580	4,122	4,122	4,580	5,954	6,412
TR158	3,916	4,895	5,385	3,427	0	4,895	3,916	4,406	4,406	4,895	7,832
TR570	5,632	5,632	7,168	4,096	4,608	0	4,096	4,608	4,608	5,632	7,168
TR144	4,433	5,910	5,910	2,463	5,418	7,388	0	3,448	4,925	6,895	6,403
TR130	5,841	7,434	7,434	3,717	6,372	7,965	3,717	0	5,310	9,558	8,496
TR147	3,512	3,951	3,951	3,512	4,390	5,268	3,512	4,829	0	3,073	7,024
F5811	3,272	3,272	3,272	3,272	4,090	4,908	4,090	4,908	3,272	0	6,544
HX100	5,750	8,050	8,050	4,600	6,900	8,625	4,600	6,325	5,750	8,050	0

These practical issues can be dealt with within the design procedure, as shown in the design example below.

A Complex Supply Chain System Design

From the results of the above optimization solution, we can suggest an easy optimal design procedure for the batch-storage networks that can be used for complex production, inventory, and distribution systems:

(1) Calculate all cycle time ratios and optimal average material flow rates for materials passing through the processes and storage units by solving the second level optimization problem in Table 1. Average material flow rates can be determined by other methods, such as linear programming, without damaging the optimality of the other variables.

(2) Identify all storage units connected to the task n in process i, as shown in Figure 6. Recycling of products to feedstock storage units is allowed. Prepare necessary input data, such as feedstock composition, product yield, storage operation time fractions, setup (or change-over) costs, inventory holding costs, capital costs and average material flow rates. The optimal batch size of task n in process i is calculated using the following equation derived from Eq. 13

$$B_{in} = \omega_i y_{in} \sum_{j=1}^{|J|} F^j_{in} = y_{in} \sum_{j=1}^{|J|} F^j_{in} \sqrt{\frac{\sum_{n'=1}^{|N(i)|} A_{in'}}{\sum_{j=1}^{|J|} \sum_{n'=1}^{|N(i)|} [a_{in'} y_{in'} F^j_{in'} + (0.5H^j + b^j)\{F^j_{in'}(1 - {}^{\backprime}x_{in'} y_{in'}) y_{in'} + G^j_{in'}(1 - x'_{in'} y_{in'}) y_{in'}\}]}} \quad (22)$$

The optimal lot size for raw material purchase is calculated using Eq. 12.

(3) Identify all processes connected to storage unit j, as shown in Figure 7. Subset $I' \subseteq I$ represents the set of supply processes, and subset ${}^{\backprime}I \subseteq I$ represents the set of consumption processes. Some materials are recycled and ${}^{\backprime}I \cap I' \neq \emptyset$. Production and inventory or supply chain systems are commonly arranged stage by stage from raw materials to finished products. 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 Eq. 18

$$\sum_{k=1}^{|K(j)|} D^j_k t^j_k - \sum_{m=1}^{|M(j)|} D^j_m t^j_m + \sum_{i=1}^{|I'|} \sum_{n=1}^{|N(i)|} G^j_{in} y_{in} t'_{in} - \sum_{i=1}^{|{}^{\backprime}I|} \sum_{n=1}^{|N(i)|} F^j_{in} y_{in} {}^{\backprime}t_{in} = V^j(0) - \sum_{m=1}^{|M(j)|} (1 - x^j_m) D^j_m \omega^j_m - \sum_{i=1}^{|{}^{\backprime}I|} \sum_{n=1}^{|N(i)|} \times (1 - {}^{\backprime}x_{in} y_{in}) F^j_{in} y_{in} \omega_i \quad \forall j \quad (23)$$

The optimal size of storage unit j is calculated using Eq. 20.

HDPE Plant Design Examples

Single reactor case

We now consider a semi-continuous process with a single reactor that produces 11 grades of HDPE. Table 2 shows the grade transition (change-over) costs ($A^{jj'}$) from column grade to row grade. These costs were estimated from the value of off-spec materials produced during grade transition. Table 3 lists the product demand rates (D^j_m), cycle time ratios (y_{in}), and inventory holding costs (H^j). Note that the cycle time ratios are known constants and are easily computed from the demand ratios because the system has only one reactor. Capital costs associated with the processes and storage units (or warehouses) are ignored for simplicity. Inventory holding costs associated with feedstock materials and the prices of materials are also ignored for simplicity. The production sequence is determined so as to minimize the sum of grade transition costs for one common production cycle and is shown in Table 3. (This problem corresponds to the traveling sales problem with 11 cities.) Note that a product is produced once within one common cycle. Eq. 15 is simplified into $\Psi_i = 0.5 \sum_{j=1}^{|J|} \sum_{n=1}^{|N(i)|} H^j y_{in}(1 - y_{in})$. Then, Eq. 13 gives a common cycle time

$$\omega = \sqrt{\frac{(41873)}{(275575)(34.96715)}} \approx 24 \text{ Days}$$

Table 3. Input and Output Data of Single Reactor Design

Sequence	Product Code	$A^{jj'}$ ($/batch)	D^j_m (ton/day)	y_{in}	H^j ($/ton/day)	$0.5H^j y_{in}(1 - y_{in})$ ($/ton/day)	B_{in} (ton)
1	F5502	2,040	30,587	0.1110	84.32	4.1598	1,792
2	F607LD	2,408	2,920	0.0106	85.41	0.4477	190
3	F6060P	2,895	5,913	0.0215	86.14	0.9043	381
4	F5811	6,544	7,665	0.0278	87.24	1.1795	491
5	HX100	4,600	2,847	0.0103	96.73	0.4945	186
6	TR144	3,448	90,885	0.3298	86.14	9.5199	4,015
7	TR130	3,717	33,580	0.1219	89.79	4.8040	1,944
8	F50100	3,206	16,571	0.0601	85.78	2.4239	1,027
9	TR158	4,895	14,454	0.0525	84.68	2.1043	903
10	TR570	4,608	11,753	0.0426	85.05	1.7362	742
11	TR147	3,512	58,400	0.2119	86.14	7.1931	3,034
Sum=		41,873	275,575	1		34.9671	

The storage sizes ($\overline{\overline{V}}^j$) are computed using Eq. 18, under the assumption of constant customer demand. Finished products are packaged and stored in a warehouse whose size is the sum of the storage sizes of all products

$$\sum_{j=1}^{|J|} \overline{\overline{V}}^j = 1792.499*(1 - 0.110993) + 190.4467*(1 - 0.010596) + 381.4212*(1 - 0.021457) + 491.2225*(1 - 0.027815) + 185.7353*(1 - 0.010331) + 4015.252*(1 - 0.329801) + 1943.857*(1 - 0.121854) + 1026.674*(1 - 0.060133) + 902.8322*(1 - 0.05245) + 741.7148*(1 - 0.042649) + 3033.89*(1 - 0.211921) = 12136 \text{ tons}$$

Two-Reactor case

We now re-cast the problem for the two-reactor case. We set the production rates of the two reactors to be equal based on savings achieved by constructing identical reactors. Solving the non-convex MINLP model in Table 1 is highly costly; hence, we introduce an easy near-optimal procedure. First, each product is allocated to either of the reactors, except the product with the largest demand (TR144). Products can be allocated to the reactors in various ways. To reduce the total change-over cost, we first adjust the single reactor production sequence to place TR144 in the middle of the sequence, and then we divide the production sequence at the location of TR144, as shown in Table 4. Note that both reactors have the same production rate. Because TR144 has the largest demand, its production can be easily split between the reactors. Then, the rest of the calculation procedure for each reactor is the same as for the single reactor case, as summarized in Table 4. The optimal cycle times of the two reactors are

$$\omega_1 = \sqrt{\frac{(22386)}{(137787.5)(31.54842)}} \approx 26 \text{ Days}$$

$$\omega_2 = \sqrt{\frac{(22920)}{(137787.5)(23.15767)}} \approx 31 \text{ Days}$$

Note that the reactors have different optimal cycle times. However, it may be desirable for both reactors to have the same cycle times in spite of the associated cost increase. This can be achieved by slightly modifying the optimization problem to give the following single cycle optimal solution

$$*\omega = \sqrt{\frac{\sum_{i=1}^{|I''|} \sum_{n=1}^{|N(i)|} A_{in}}{\sum_{i=1}^{|I''|} \Psi_i(F^j_{in}, G^j_{in}, y_{in})}} \quad I'' \subseteq I \tag{21}$$

Table 4. Input and Output Data of Two-Reactor Design

Process	Sequence	Product	$A^{jj'}$ ($/batch)	y_{in}	H^j ($/ton/day)	$0.5H^j y_{in}(1 - y_{in})$ ($/ton/day)	D^j_m (ton/day)	B_{in} (ton)
R1	1	TR130	3,717	0.2437	89.79	8.2748	33,580	2,410
R1	2	F50100	3,206	0.1203	85.76	4.5365	16,571	1,189
R1	3	TR158	4,895	0.1049	84.68	3.9756	14,454	1,037
R1	4	TR570	4,608	0.0853	85.05	3.3177	11,753	11,340
R1	5	TR147	3,512	0.4238	86.14	10.518	58,400	4,191
R1	6	TR144	3,448	0.0220	86.14	0.9261	3,029.5	217
Sum=			22,386	1		31.548	137,788	
R2	1	TR144	4,433	0.6376	86.14	9.9518	87,855.5	7,446
R2	2	F5502	2,040	0.2220	84.32	7.2810	30,587	2,592
R2	3	F607LD	2,408	0.0212	85.41	0.8858	2,920	247
R2	4	F6060P	2,895	0.0429	86.14	1.7690	5,913	501
R2	5	F5811	6,544	0.0556	87.24	2.2914	7,665	650
R2	6	HX100	4,600	0.0207	96.73	0.9786	2,847	241
Sum=			22,920	1		23.1577	137,788	

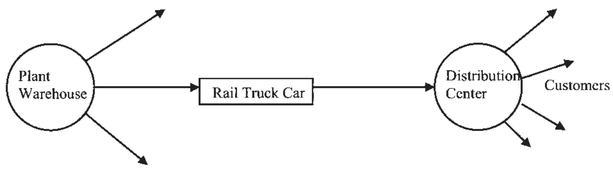

Figure 8. An example product distribution branch.

where the cycle times of process subset I'' are the same. The value of the optimal cycle time for this example is as follows

$$\omega = \sqrt{\frac{(45306)}{(137787.5)(54.70609)}} \approx 28 \text{ Days}$$

Note that the optimal cycle times for the two-reactor system are longer than that of the single reactor system, mainly due to the increase in total change-over (grade transition) cost on introducing a second reactor. Note also that we used the grade transition cost data in Table 2, which were collected from a two-reactor system for both cases. The grade transition cost is usually proportional to the volume of off-spec product during grade transition. Under the assumption of constant grade transition time, the grade transition costs of a higher flow rate reactor are greater than those of one with a lower flow rate. If we assume that the grade transition cost is proportional to the average flow rate, the common cycle time for the single reactor case should be changed to $\sqrt{2}*24 \approx 34$ days. Note that the task batch size of TR144 on reactor 1 is very small and is probably smaller than the minimum batch size for TR144. Thus, a portion of the TR144 production should be moved from reactor 2 to reactor 1. To balance the production of the two reactors and meet the minimum production volume, another product may be produced on both reactors.

We additionally attempted to solve the above design problems by using a mathematical programming technique. Specially, the second level optimization problem in Table 1 was programmed and solved with the commercial software GAMS/DICOPT++. However, despite repeated trials, the solutions of the non-convex MINLP problem obtained using this approach were worse than the above results.

Transportation and distribution facilities

Figure 8 shows an example product distribution branch of an HDPE plant. The products in the plant warehouse are transported by rail truck car (RTC) to a distribution center (DC). We assume that the customer demand of this DC is exactly 30% of the total demand in Table 3 for each product. Customers place orders on weekdays, and there is no shipping on weekends. The fixed charge cost of transportation by RTC between the plant warehouse and DC is $50,000. For simplicity, we ignore all other costs except inventory holding cost, that is, $a_{in} = b^j = 0$. The transportation process is a single task; hence $|N(i)| = y_{in} = 1$. The storage operation time fraction of each RTC is assumed to be 0.9. The optimal capacities of the RTC and DC are computed using Eqs. 20 and 22:

$$\Psi_{RTC} = 2*0.5*0.3*(1-0.9)(30587*84.315 + 2920*85.41 + 5913*86.14 + 7665*87.235 + 2847*96.725 + 90885*86.14 + 33580*89.79 + 16571*85.775 + 14454*84.68 + 11753*85.045 + 58400*86.14) = 2380115.251$$

$$B_{RTC} = (0.3*275575)\sqrt{\frac{50000}{2380115.251}} = 11982 \text{ tons}$$

$$\bar{\bar{V}}^{DC} = 11982.49*(1-0.9) + (0.3*275575)*7*(1-5/7) = 166543 \text{ tons}$$

Note that the plant warehouse size in Tables 3 and 4 does not reflect the effect of RTC and, therefore, the warehouse size should be increased by 11982 * (1− 0.9).

Conclusions

An analytical solution for the optimal lot sizing of multitasking batch or semi-continuous processes with variable feedstock composition and product yield has been developed within the framework of a batch-storage network. The method presented here makes it possible to apply the PSW model to diverse chemical processes, including those that produce major commodity chemicals, such as fuel oils, petrochemicals, polymers, solvents, and lubricants, as well as those producing specialty chemicals. The applicability of the PSW model was widened to include these chemical processes by assuming a fixed periodic production task sequence. Thus, the proposed method is useful for processes with a limited number of feasible production sequences, each of which has a different total setup or change-over cost. The cycle time ratios are assumed to be known constants, which is valid for single process systems and multi-process systems without split production. For general multi-process systems, the cycle time ratios are treated as variables, and Eq. 19 becomes a highly nonlinear objective function. The resulting non-convex mixed integer optimization problem requires a huge amount of computation and is, therefore, expensive to solve; future work should, therefore, aim to find a tractable solution to this problem. In the present study, we suggested an easy near-optimal procedure that can be used for most practical design problems, as demonstrated by applying the procedure to the problem of designing an HDPE plant. Additionally, we suggested a practical process optimality measure that is applicable to any kind of process. It is noteworthy that this optimality measure is not derived empirically but rather from the batch-storage network optimization model. This measure can be exploited to efficiently allocate organization resources in a manner that ensures global enterprise optimality.

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Notation

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

a_{in} = annualized capital cost of process i, task n, dollars per unit of item per year

b^j = annualized capital cost of storage facility, dollars per unit of item per year
A_k^j = ordering cost of feedstock materials, dollars per order
A_{in} = ordering cost of noncontinuous process i, task n, dollars per order
$A^{jj'}$ = product change-over cost from product j to product j', dollars per order
B_k^j = raw material order size, unit of items per lot
B_{in} = noncontinuous process size, unit of items per lot
B_m^j = final product delivery size, unit of items per lot
D_k^j = average material flow of raw material supply, unit of items per year
D_m^j = average material flow of customer demand, unit of items per year
D_i = average material flow through noncontinuous processes, unit of items per year
f_{in}^j = feedstock composition of process i, task n
F_{in}^j = average flow rate of feedstock material j to process i, task n, unit of items per year
g_{in}^j = product yield of process i, task n
G_{in}^j = average flow rate of product material j from process i, task n, unit of items per year
H^j = annual inventory holding costs, dollars per unit of item per year
I = noncontinuous process set
I' = supply process subset
$`I$ = consumption process subset
I'' = process subset with the same cycle time
J = storage set
$K(j)$ = raw material supplier set for storage j
$M(j)$ = consumer set for storage j
$N(i)$ = task set for process i
P_k^j = price of raw material j from supplier k, \$/units of item
P_{in}^j = price of processing material j in process i and task n, \$/units of item
t_m^j = start-up time of customer demand, year
$`t_i$ = start-up time of the first task feedstock feeding to noncontinuous process i, year
$`t_{in}$ = start-up time of feedstock feeding of task n to noncontinuous process i, year
t'_{in} = start-up time of product discharging of task n from noncontinuous process i, year
t_k^j = start-up time of raw material purchasing, year
$\underline{\underline{V}}^j$ = upper bound of inventory hold-up, units of item
$\bar{\bar{V}}^j$ = lower bound of inventory hold-up, units of item
$V^j(t)$ = inventory hold-up, units of item
$V^j(0)$ = initial inventory hold-up, units of item
$\bar{V}^j$ = time averaged inventory hold-up, units of item
x_k^j = storage operation time fraction of purchasing raw materials
$`x_{in}$ = storage operation time fraction of feeding to noncontinuous process i, task n
x'_{in} = storage operation time fraction of discharging from noncontinuous process i, task n
x_m^j = storage operation time fraction of customer demand
y_{in} = cycle time ratio, ω_{in}/ω_i
Y_{in}^l = binary variable to linearize y_{in} in piece-wise manner
$Z_{in}^{jj'}$ = Z_{in}^{jj} = 1 if the n-th task on process i produces a product j and the (n + 1)-th task produces a product j' and otherwise, $Z_{in}^{jj'} = 0$

Greek letters

$\underline{\underline{\theta}}$ = physical property of product storage
$\underline{\underline{\theta}}^j$ = physical property of feedstock storage j
$\underline{\underline{\lambda}}^j$ = Lagrangian multipliers
$\phi^{jj'}$ = the composition of feedstock j to produce product j'
ω_m^j = cycle time of customer demand, year
ω_k^j = cycle time of raw material purchasing, year
ω_i = common cycle time of noncontinuous process i, year
ω_{in} = duration of task n of noncontinuous process i, year
Ψ_i = aggregated cost defined by Eq. 15
Ψ_k^j = aggregated cost defined by Eq. 14

Subscripts

i = noncontinuous process index
k = raw material vendors
m = finished product customers
n = task index

Superscripts

j = storage index
l = dummy index l=0, 1, . . . ,L

Special Functions

int[.] = truncation function to make integer
res[.] = positive residual function to be truncated
$|X|$ = number of elements in set X

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Appendix A: Kuhn-Tucker Solution to the First Level Optimization Problem

The start-up time $`t_{in}$ and $t'_{in}$ is converted into $`t_i$ by Eqs. 2 and 3. Eq. 10 can be transformed into the following expression in terms of the independent variables by using Eqs. 7 and 9

$$TC = \sum_{j=1}^{|J|}\sum_{k=1}^{|K(j)|}\left[\frac{A_k^j}{\omega_k^j}\right] + \sum_{i=1}^{|I|}\left[\frac{\sum_{n=1}^{|N(i)|} A_{in}}{\omega_i}\right] + \sum_{j=1}^{|J|}\sum_{k=1}^{|K(j)|}\left[\left(\frac{H^j}{2} + b^j\right)\right.$$

$$\left.\times (1 - x_k^j) + a_k^j\right] D_k^j\omega_k^j - \sum_{j=1}^{|J|}\sum_{k=1}^{|K(j)|}(H^j + b^j)\, D_k^j t_k^j$$

$$+ \sum_{i=1}^{|I|}\omega_i \sum_{n=1}^{|N(i)|}\sum_{j=1}^{|J|} a_{in}F_{in}^j y_{in} + \sum_{j=1}^{|J|}\left(\frac{H^j}{2} + b^j\right)\sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}(1$$

$$- x'_{in}y_{in})G_{in}^j y_{in}\omega_i - \sum_{j=1}^{|J|}(H^j + b^j)\sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}\Delta t_{in}G_{in}^j y_{in}$$

$$- \sum_{j=1}^{|J|}\frac{H^j}{2}\sum_{i=1}^{|I|}\sum_{n=1}^{|N(i)|}(1 - `x_{in}y_{in})\, F_{in}^j y_{in}\omega_i + \sum_{J=1}^{|J|}(H^j$$

$$+ b^j) \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \left(\sum_{n'=1}^{n-1} y_{in'} \right) (F_{in}^j - G_{in}^j) y_{in} \omega_i + \sum_{j=1}^{|J|} (H^j + b^j) \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (F_{in}^j - G_{in}^j) y_{in} \backprime t_{in} \quad \text{(A1)}$$

$+$ constants

$$\text{constants} = \sum_{j=1}^{|J|} (H^j + b^j) V^j(0) - \sum_{j=1}^{|J|} \sum_{m=1}^{|M(j)|} \left(\frac{H^j}{2} \right) (1 - x_m^j) D_m^j \omega_m^j + \sum_{j=1}^{|J|} \sum_{m=1}^{|M(j)|} (H^j + b^j) D_m^j t_m^j \quad \text{(A2)}$$

The Lagrangian for the optimization problem to minimize Eq. 10 subject to Eq. 11 with respect to ω_k^j, ω_i, t_k^j, and $\backprime t_i$ is

$$L = TC - \sum_{j=1}^{|J|} \underline{\underline{\lambda}}^j \Bigg[V^j(0) - \sum_{k=1}^{|K(j)|} D_k^j t_k^j + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (F_{in}^j - G_{in}^j) y_{in} \backprime t_i + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \left(\sum_{n'=1}^{n-1} y_{in'} \right) (F_{in}^j - G_{in}^j) y_{in} \omega_i - \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \Delta t_{in} G_{in}^j y_{in} - \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (1 - \backprime x_{in} y_{in}) F_{in}^j y_{in} \omega_i - \sum_{m=1}^{|M(j)|} (1 - x_m^{in}) D_m^j \omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j \Bigg] \quad \text{(A3)}$$

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

$$\frac{\partial L}{\partial t_k^j} = -(H^j + b^j) D_k^j + \lambda_{lb}^j D_k^j = 0 \quad \text{(A4)}$$

$$\frac{\partial L}{\partial \omega_k^j} = -\frac{A_k^j}{(\omega_k^j)^2} + \left[\left(\frac{H^j}{2} + b^j \right) (1 - x_k^j) + a_k^j \right] D_k^j = 0 \quad \text{(A5)}$$

$$\frac{\partial L}{\partial t_i} = \sum_{j=1}^{|J|} (H^j + b^j) \sum_{n=1}^{|N(i)|} (F_{in}^j - G_{in}^j) y_{in} - \sum_{j=1}^{|J|} \lambda^j \sum_{n=1}^{|N(i)|} (F_{in}^j - G_{in}^j) y_{in} = 0 \quad \text{(A6)}$$

$$\frac{\partial L}{\partial \omega_i} = -\frac{\sum_{n=1}^{|N(i)|} A_{in}}{(\omega_i)^2} + \sum_{n=1}^{|N(i)|} \sum_{j=1}^{|J|} a_{in} F_{in}^j y_{in} + \sum_{j=1}^{|J|} \left(\frac{H^j}{2} + b^j \right) \sum_{n=1}^{|N(i)|} (1 - x'_{in} y_{in}) G_{in}^j y_{in} - \sum_{j=1}^{|J|} (H^j + b^j) \sum_{n=1}^{|N(i)|} G_{in}^j y_{in} \frac{\partial \Delta t_{in}}{\partial \omega_i} - \sum_{j=1}^{|J|} \frac{H^j}{2} \sum_{n=1}^{|N(i)|} (1 - \backprime x_{in} y_{in}) F_{in}^j y_{in} + \sum_{J=1}^{|J|} (H^j + b^j) \sum_{n=1}^{|N(i)|} \left(\sum_{n'=1}^{n-1} y_{in'} \right) (F_{in}^j - G_{in}^j) y_{in} - \sum_{j=1}^{|J|} \underline{\underline{\lambda}}^j \left[\sum_{n=1}^{|N(i)|} \left(\sum_{n'=1}^{n-1} y_{in'} \right) (F_{in}^j - G_{in}^j) y_{in} - \sum_{n=1}^{|N(i)|} G_{in}^j y_{in} \frac{\partial \Delta t_{in}}{\partial \omega_i} - \sum_{n=1}^{|N(i)|} (1 - \backprime x_{in} y_{in}) F_{in}^j y_{in} \right] = 0 \quad \text{(A7)}$$

$$\underline{\underline{\lambda}}^j \Bigg[V^j(0) - \sum_{k=1}^{|K(j)|} D_k^j t_k^j + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (F_{in}^j - G_{in}^j) y_{in} \backprime t_i + \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \times \left(\sum_{n'=1}^{n-1} y_{in'} \right) (F_{in}^j - G_{in}^j) y_{in} \omega_i - \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} \Delta t_{in} G_{in}^j y_{in} - \sum_{i=1}^{|I|} \sum_{n=1}^{|N(i)|} (1 - \backprime x_{in} y_{in}) F_{in}^j y_{in} \omega_i - \sum_{m=1}^{|M(j)|} (1 - x_m^{in}) D_m^j \omega_m^j + \sum_{m=1}^{|M(j)|} D_m^j t_m^j \Bigg] = 0 \quad \text{(A8)}$$

Solving Eqs. A4 and A6 gives

$$\underline{\underline{\lambda}}^j = H^j + b^j \quad \text{(A9)}$$

Solving Eqs. A5 and A7 with Eq. A9 gives Eqs. 12 and 13 in the main text. Solving Eq. A8 gives Eq. 18 in the main text.

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