AC 2010-726: A MODULE FOR TEACHING BATCH OPERATIONS

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A Module for Teaching Batch Operations

Rationale

For the past several years, the majority of projects chosen for one of the two required designs in our senior capstone course have involved some form of batch or semi-batch process. However, no formal instruction in the design and operation of batch processes was covered in the lecture portion of the senior design course. Only a few of the basics of batch operations might be covered in an undergraduate curriculum; unsteady material and energy balances (Stoichiometry and Heat Transfer), design of batch reactors (Chemical Reaction Engineering) and control of simple batch operations such as tank filling, etc. (Process Control). To complement the coverage of batch operations and to familiarize students with additional concepts relating to batch operations such as scheduling and intermediate storage, a short module in batch operation was developed for a senior design course.

Integration of Batch Operations into the Existing Senior Design Curriculum

The senior design course at our University comprises two semesters. The first semester includes 3 hours of lectures per week; a year-long, group design project (often batch/semi-batch); and an individual design project (traditional, continuous chemical process). The second semester comprises the continuation of the group design project and a second individual design project. Three hours of lecture were added to the fall semester to provide an introduction to batch processing.

This module is presented early in the semester, immediately following the presentation of the "hierarchical approach to process design" that follows the approach of Douglas[1]. The first step in this hierarchy is the choice between batch and continuous operation. We follow this discussion with the batch-processing module, and then follow this with continuous-process flowsheet analysis.

Batch Topics Covered in Module

A comprehensive coverage of batch processes cannot be accomplished in 3 hours of lecture. So, the issue is what to include in an introduction to the topic. Within the constraints of the 3 allotted hours, the following topics are given priority and are discussed in detail:

- Formulation of basic recipes
- Equipment design
- Gantt charts and scheduling
- Single- and multi-product processes
- Cycle times
- Intermediate and product storage
- Basic optimization of batch processes
- Use of process simulators

Recipes: Virtually all operations in batch processes follow specific procedures or recipes. These recipes may be very specific, as might be the case for a pharmaceutical processes in which strict adherence to good manufacturing practices (GMP) is required for all steps in the production of the product. On the other hand, the recipe might be less formalized and involve some "art" as in the case of producing a batch of special colored glass. An example of a recipe to produce a chemical product is shown in Table 1, where only details of the first two steps are given. The key elements of a recipe are the time required for each step, the equipment used, and the raw materials and utilities required.

Table 1: An example of a recipe for producing a chemical product[2]

Step	Procedure
1	500 kg of reactant A (MW = 100 kg/kmol) is added to 5000 kg of a mixture of organic solvent (MW = 200 kg/kmol) containing 60% excess of a second reactant B (MW = 125 kg/kmol) in a jacketed reaction vessel (R-301), the reactor is sealed, and the mixture is stirred and heated (using steam in the jacket) until the temperature has risen to 95°C. The density of the reacting mixture is 875 kg/m3 (time taken = 1.5 h).
2	Once the reaction mixture has reached 95°C, a solid catalyst is added, and reaction takes place while the batch of reactants is stirred. The required conversion is 94% (time taken = 2.0 h).
3	…………………………………………………………………………………
4	…………………………………………………………………………………
5	…………………………………………………………………………………

Equipment Design: A brief review of unsteady state operations is given and examples of physical operations (heating, cooling, or mixing) are covered. The relationship between time in a batch reaction and length in a plug flow reactor is reviewed. The difficulty in recycling material and integrating energy in batch processes are explained and the importance of material transfer and equipment cleaning are emphasized. Another important consideration when sizing batch equipment is that normally it is available in a limited number of predetermined standard sizes. Therefore, batch processes are tailored to fit the equipment unlike in continuous processes when equipment is designed, most often, specifically for the process. The specifics of equipment design and simulation for other batch unit operations (distillation, filtration, crystallization, etc.) are not covered but are left for specific operations related to the group project.

As an example of the differences between unsteady, batch operation and continuous operation, consider the preheating of a batch reactor with preheating of a continuous reactor in a continuous heat exchanger. The familiar, steady-state equations for a heat exchanger are the energy balances and the heat-exchanger design equation (assuming a utility of condensing steam, for example)

$$Q = \dot{m}_p C_{p,p} \Delta T_p = \dot{m}_s \lambda_s = UA\Delta T_{lm} F \tag{1}$$

where the subscript p represents the process stream, and the subscript s represents the steam utility. For heating in a well-mixed, batch tank with a heating coil or jacket, the unsteady energy balance is

$$\rho V C_p \frac{dT}{dt} = UA(T_s - T) = \dot{m}_s \lambda \tag{2}$$

where ρ is the liquid density, V is the volume of liquid in the tank, C_p is the liquid heat capacity, T is the temperature of the liquid in the tank, U is the overall heat transfer coefficient from the jacket or coil, A is the heat transfer area of the jacket or coil, and T_s is the temperature of the condensing steam utility. Integration of this equation yields

$$\ln \frac{(T_s - T)}{(T_s - T_o)} = -\frac{UAt}{\rho V C_p} \tag{3}$$

where T_o is the initial temperature in the tank.

In the continuous case, if all physical properties are known, for a desired process-outlet temperature, the amount of steam and heat-exchanger area can be calculated. For the batch process, time is an additional variable. For a desired final temperature, the heat transfer area and heating time are inversely related. A larger area requires less heating time and vice-versa. Therefore, an additional decision variable is introduced into the batch design optimization. This simple example illustrates one of the differences between modeling, design, and optimization procedures for batch and continuous operations. Another constraint in batch modeling is that the volume of the batch must be matched with the equipment size. This imposes additional constraints on Equation 3. For example, not all combinations of t and A can be accommodated, if t is small and A is large, the volume of process liquid may be too small to cover the coil or jacket.

Gantt charts and scheduling: The scheduling of different equipment in a given process is best illustrated through the use of simple Gantt charts. Gantt charts are used extensively in the scheduling and planning of all sorts of projects[3], and can become very complicated and require significant experience to interpret. However, they can be used in batch processes to give a simple pictorial representation of the timing of events and use of equipment. Figure 1, shows the equipment usage for the recipe given in Table 1. For this example, the total time to complete one batch (cycle time) is 14.5 hours.

Single- and multi-product processes: Most often, a batch processing facility will produce a variety of products. The schedule by which each product is manufactured depends on several factors including demand, availability of product storage, and transportation needs. In general, batch operations involve running "campaigns," in which either a single product or a mixture of products is produced. When a single product is produced, a campaign will consist solely of that product. The production schedule will look like that shown in Figure 2, and the equipment with the longest process time is the rate-limiting step, for this case the dryer is limiting and the cycle time is 4 h.

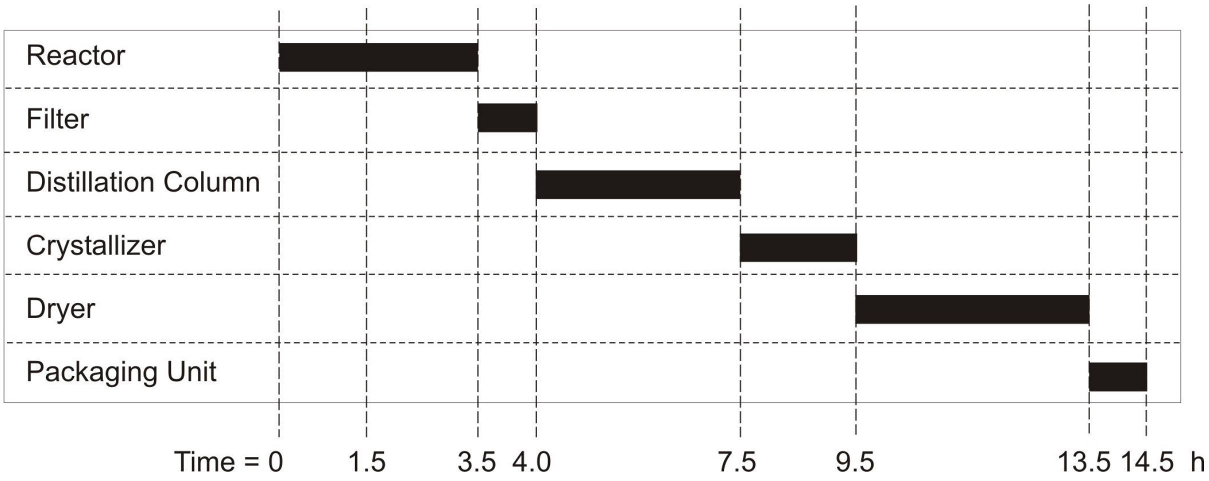

Figure 1: A Gantt Chart for the Process Shown in Table 2[2]

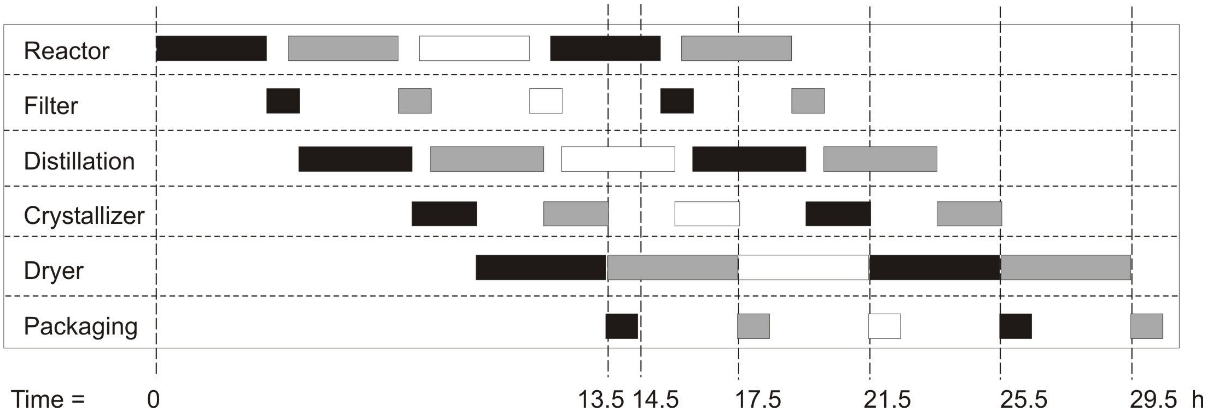

Figure 2: Sequencing of Operations in a Single-Product Campaign[2]

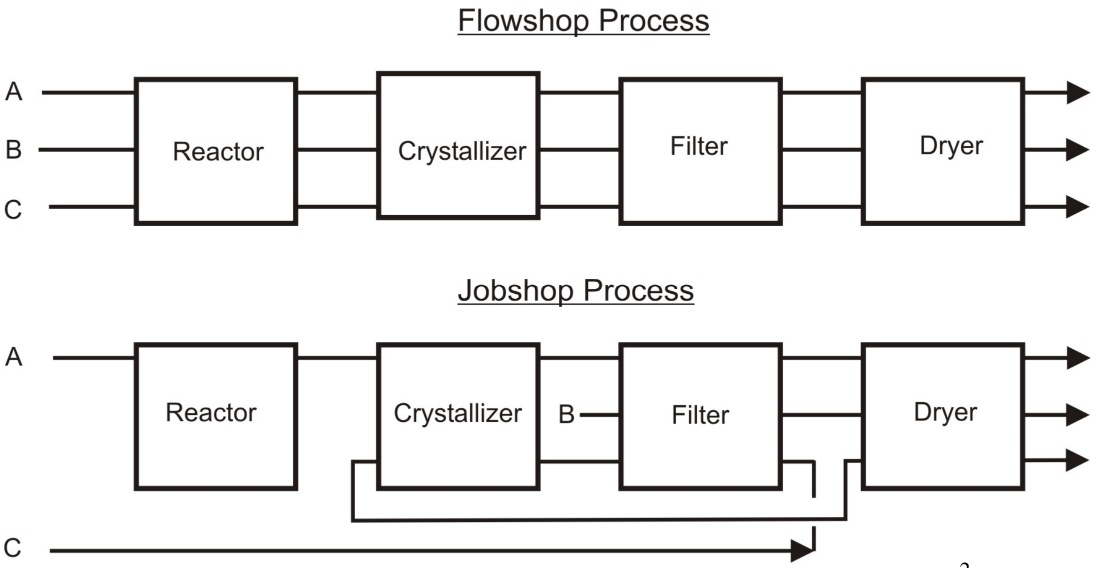

Figure 3: Flow of Material through Flowshop and Jobshop Plants[2]

For multi-product processes, the scheduling can take place as separate, single-product campaigns following each other or campaigns in which each product is produced a number of times, *e.g.*, ABCCABCCABCC. The situation for multi-product production processes is further complicated depending on the sequence of equipment needed to produce each product. If all products use the same equipment in the same sequence (but for different times), the process is called a Flowshop process.[4] Otherwise, the process is called a Jobshop process. Flowshop and Jobshop processes are illustrated in Figure 3.

Cycle times: The cycle time is simply the minimum time needed to repeat the batch. For single product campaigns:

$$t_{cycle} = \max_{i=equip}[t_i] \tag{4}$$

Therefore, the cycle time is the maximum processing time of the times in each piece of equipment in the processes. For the example shown in Figure 1, the cycle time is 4 h and equal to the processing time for the dryer. For multiple products using single product campaigns, *e.g.*, make all A, then B, then C, the cycle times are additive:

$$t_{cycle,total} = t_{cycle,A} + t_{cycle,B} + t_{cycle,C} \tag{5}$$

For multi-product campaigns and flowshop processes, *e.g.*, ABCABCABCABC…., the cycle time is given as follows:

$$t_{cycle} = \max_{i=equip} \sum_{j=processes} t_{i,equip} \tag{6}$$

For multi-product campaigns and jobshop processes, the situation is more complicated and is discussed elsewhere.[2]

Intermediate and product storage: If single-product campaigns are used for a multi-product plant and demand for each product is constant, then some amount of product storage will be required to provide a constant supply of each product. If a campaign takes place over some time, t_{camp}, and the rate of production during that campaign is r_p and the rate of demand is r_d, then the minimum product storage, V_p is given by:

$$V_p = (r_p - r_d)t_{camp} \tag{7}$$

Intermediate storage is helpful in reducing bottlenecks and can decrease the cycle time for multi-product sequencing at the expense of the additional storage and additional material transfer costs. If unlimited intermediate storage is available then cycle times are minimized. An example of improved cycle times will be discussed in the presentation.

Basic optimization of batch processes: One of the big differences between optimization of continuous processes and batch processes is the need to include the time variable in the batch optimization. For example, for a simple first-order reaction occurring in a batch reactor, what is the optimal run time for the reactor? The trade-offs are loss of conversion vs. size of reactor. However, since the reactor would have to be cleaned between batches, the clean-up time, t_{clean}, must also be considered. When dealing with multiple products, the profit from each product must be weighed against the time needed to make the product (t_{cycle}). For multiple single-product campaigns with linear constraints, the optimum product mix can be formulated and solved relatively easily. However, there are many issues associated with the general optimization batch problems and their solution becomes very complicated and requires techniques beyond the scope of the current module.

Problem Assignments: Problem assignments focus mostly on batch scheduling. When teaching optimization, the costs associated with cleaning, alternative scheduling patterns, and alternative product mixes are included.

Use of process simulators: The common process simulators (AspenPlus (http://www.aspentech.com), Hysys (http://www.aspentech.com), Chemcad (http://www.chemstations.com), PRO/II (http://www.simsci.com) can be used to simulate various batch operations and are very useful when "conventional" chemical processes are being used. For these processes, the use of sophisticated thermodynamic models is often essential to model the unit operations taking place accurately. However, for many biological processes, the reactant medium can often be modeled accurately as water. The engineer is often interested in keeping track of multiple trace ingredients used as buffering agents in the media, and the reactions taking place often involve the production of biomass of undetermined molecular structure. For such cases, it is often easier to do basic material and energy balance equations using a spreadsheet or a simulator designed specifically for these types of process such as SuperPro Designer and SchedulePro by Intelligen, Inc. (http://www.intelligen.com). A discussion of the pros and cons of different modeling approaches will be covered in the presentation.

Conclusions

The three-hour module developed for the senior design class covers the basics of batch processes, with the emphasis on the scheduling of equipment for single- and multiple-product plants. The material covered in the module is meant to supplement what might be taught in the first three years of the traditional undergraduate curriculum. Mastery of the material in the module gives students a familiarity with the nomenclature associated with batch processes and a basic understanding of many key issues associated with batch processing.

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