A GENERAL PROCEDURE FOR THE SYNTHESIS OF PROCESS FLOWSHEETS

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Abstract

The research was divided into two parts: examining (1) continuous and (2) batch processes. The work on continuous processes was focused on the development of a more general procedure for the systematic synthesis of process flowsheets that identifies the most important process alternatives (including waste minimization alternatives), the dominant design variables, and the minimum energy consumption for each alternative for continuous, vapor-liquid-liquid-solid processes for the production of nonpolymeric materials. The work was an extension of the hierarchical synthesis procedure previously developed for vapor-liquid processes. A new superstructure for continuous process flowsheets, along with an extended set of rules for the classification of components, with special attention to waste minimization, and solvent selection was developed. The work on batch processes was focused on the development of new procedures for the design and scheduling of multiproduct batch plants. The approach was based on simulated annealing and the solution of the optimal sequencing problem as well as the results on the design problem are described in this report.

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1. Synthesis of Continuous Process

In order to extend the synthesis procedure for continuous vapor/liquid processes to vapor-liquid-liquid-solid systems, a new superstructure for a continuous process flowsheet was required. The synthesis rules for the feed streams and exit streams for the process are largely unchanged, except for a more detailed classification of waste streams. Similarly, the synthesis rules for the reactor recycle streams remained intact except when there is a need for reactor solvents. However, a completely new superstructure was developed for the synthesis of the separation system. Each of these areas is described below. The results for waste minimization problem have been published and a manuscript for the separation system synthesis is attached.

1.1 Flowsheet Superstructure

The new superstructure we have developed for a continuous process flowsheet is shown in Fig. 1. New rules were developed for specifying which general separations operations are required, for selecting the particular units (as well as their alternatives) that can be used for each of the separations, and the development of short-cut design and cost equations for each of the units. In addition, new techniques for solving the separation system material balance equations were needed, because of the large number and the coupled nature of the recycle loops. Vapor-liquid-liquid-solid processes often have large waste streams, and so design for waste minimization is a significant problem.

Figure 1. General Structure of a Continuous Flowsheet, including the vapor/liquid/liquid/solid separation system.

1.2 Component Classification for Waste Minimization: Input-Output Structure

The original synthesis procedure considered only vapor-liquid processes. Since solids were not considered, any waste streams were usually classified as waste water and sent to pollution treatment facilities. However, for vapor-liquid-liquid-solid processes, waste streams can also be sent to land fills or incinerators, as well as to bioponds. Hence, the new component classifications that can be used for vapor-liquid-liquid-solid processes are given in Table 1. These classifications are used to determine what separations are required, since components that have different destinations must be separated.

<i>Component Classification</i>	<i>Destination</i>
Reactant (liquid or solid)	Recycle
Reactant (gas)	Gas recycle & purge
Reaction Intermediate	Recycle
By-product from secondary reversible reaction	Recycle or exit
Product	Product Storage
Valuable by-product	By-product Storage
Fuel by-product	Fuel supply
Inert gaseous by-product	Vent
Aqueous waste	Biopond
Incineration waste	Incinerator
Solid waste	Land fill

Table 1. Component Classifications and Destinations

1.3 Reactor Solvents

If there is a feed component that is a solid and a liquid phase reaction takes place in the process, then it is necessary to change the phase of the feed component. When the melting point of this feed component is less than the reactor temperature, then we simply melt the feed, and recycle any of the component that is not converted in the reactor as a liquid. However, if the melting point of the feed exceeds the reactor temperature, then we must add a solvent to dissolve the solid. If we select a solvent other than water, economics indicates that we must recover and recycle the solvent (with a small loss). However, if water is used as a solvent, it has been common practice to discard the water, and a waste minimization problem is encountered.

1.4 Separation System Synthesis

After making the decisions for the Input-Output Structure (Level 2) and Recycle Structure (Level 3) we estimate the feed, exit and recycle flows using the short-cut material balance procedures developed previously (solvent recycle flows are estimated using a flow 20 % greater than that required for saturation). Since the reactor exit flows and the component destinations define the separations problem, we can synthesize a separation system. When we can phase split the reactor exit stream, we can decompose the separations problem into a vapor recovery system, a solid recovery system and one or more liquid separation systems. Hence, the first separation we consider is the phase splitting of the reactor exit stream.

1.4.1 Phase Splits

If the reactor exit stream has multiple phases and if the flows of the phases are reasonably well-balanced we split vapors in a flash drum, next we remove solids in a liquid solid separator (a filter or centrifuge, or we might need a thickener before these units), and then we split liquid phases in a decanter. For unbalanced flows we might reverse the decanter and filter operations. There are many partial oxidation processes where the product is a solid, and vapor-liquid-liquid-solid mixtures are encountered at the reactor exit.

In cases where the reactor exit stream is a vapor, we cool the reactor exit stream so that a phase split is possible. If the reactor exit stream is a liquid, we prefer to separate the mixture by distillation. However, if distillation is not feasible because of the presence of temperature sensitive materials (decompose), monomers, unstable intermediates, then we sometimes cool the reactor exit stream to crystallize one or more components in order to achieve a phase split. Alternatively, if the reactor exit stream is an organic liquid, we often add water to create a phase split, and for aqueous exit streams we often add organics. Thus, both cooling and the addition of "mass separating agents" can be used to cause phase splits.

1.4.2 Vapor Recovery System

The synthesis of the vapor recovery system does not change if we have liquid-liquid-solid mixtures leaving a flash drum. We synthesize the vapor recovery system before a liquid separation system because solvents can either be recovered locally (if an extraneous component that is either more volatile or less volatile than the other components being recovered from the gas stream is used as a solvent) or along with the separation of the

reactants, product and by-products if the solvent is a component that exits in the system.

1.4.3 Solid Recovery System

There are a large number of alternatives for liquid/solid separators and for the washing of filter/centrifuge cakes to recover valuable materials from the cake. Selection rules for the equipment have been developed, and short-cut models have been derived. In addition, synthesis rules and material balances for different crystallizer-filter/centrifuge-dryer systems (including a single crystallizer, two crystallizers in series with or without solids recycle, two crystallizers in series followed by dissolution and re-crystallization), depending on the purity specifications of a solid product, have been derived. We synthesize the solid separation system before the liquid separation system, because the recovery of valuable materials from the wash liquid can be combined with the liquid separation system that is used to separate reactants, liquid by-products, and a liquid product.

1.4.4 Liquid Separation System

The liquid separation units that have been considered include stripping, distillation, extraction, and crystallization. In some processes more than one liquid separation technique is used in the same flowsheet, e.g., in the flowsheet for the production of aminophenol shown in Fig. 2, where crystallization, distillation and extraction all are used to separate some of the components. Rules, short-cut material balances and short-cut design models have been developed for these operations.

Figure 2. Aminophenol Flowsheet

2. Batch Processes

Design and synthesis procedures have been previously developed for single-product plants with uniform average demands for a product. This is an interesting limiting case, but a much larger class of problems is faced in practice. For example, multiproduct plants with a relatively large number of products are common and distinct due dates for discrete amounts of each product are often specified. The synthesis results for a single product plant are quite inadequate to attack these batch process design problems. With the research support in this grant, we have been able to develop a design and synthesis approach more suited to batch processes. Some of the earlier work on scheduling aspects is described in DOE Progress Report No. DOE/ER/13676-6.

In the third year of support for this project, we propose to completed studies using a generalized simulated annealing approach to integrate design, scheduling and synthesis of batch processes. The results are described in several papers, which are appended to this report and summarized below.

2.1 Design of Multiproduct Plants

A new formulation for the design of multiproduct batch plants is described. In contrast to previous work, the demand is not assumed to have the form of a single aggregate due date common to all of the products. In addition, the economic objective accommodates inventory, changeover, operating, and capital costs as well as penalties for early and late production. The multiplant structure is considered to allow the simultaneous production of multiple products using different types of production lines, multiple production routes for

individual products, and parallel units at each stage. The production planning, the plant design and the flowsheet synthesis are optimized simultaneously using simulated annealing. A relatively simple case of parallel flowshops, where the optimal planning, number of production lines, and equipment sizes are determined, is treated to illustrate the impact of distinct due dates and penalties for early and late production. A more interesting and complex design problem incorporating process synthesis decisions is then examined, with different demand profiles and changeover costs. This approach provides a general and flexible framework for a variety of problems, each with different constraints, decision variables and objectives.

2.2 Effects of Uncertainties

Scheduling of multiproduct chemical plants is often based on parameter values from forecasts which are subject to high uncertainties. It will be shown that deterministic procedures, to a certain extent, can account for uncertainties in demand and batch times and generate flexible schedules. A simple simulated annealing procedure to account for uncertainties in batch times is first described; this method generates sequences either optimum in the average case, worst case, or less sensitive to batch time uncertainties. It is shown that traditional deterministic scheduling algorithms can lead to infeasible schedules when uncertainties in batch times arise in units governed by the zero-wait policy. An existing completion-time calculation algorithm is accordingly modified to overcome this problem. A simulated annealing procedure, reported in a previous study, for the sequence optimization of batches in serial units (flowshop) with an economic objective including inventory,

changeover costs as well as penalties for late deliveries is then extended to accommodate uncertainties in demand. The main advantage of the different methods outlined in this study is that they are simple and fairly general. In contrast to other studies, very little quantitative knowledge of the uncertainties is used, which will be often acceptable, since this knowledge is generally limited and unsettled.

2.4 Application to Polymer Production

The interaction of the selection of operating conditions with the global design of multiproduct batch processes is investigated with an example of production of chain-growth polymers. The simulated annealing approach developed for planning, design and synthesis in a previous study is extended to include operating conditions in the optimization. In contrast to most published work, the economic objective accommodates inventory, changeover, operating, recycle, labor and capital costs as well as penalties for early and late production. The production of polystyrene and poly(styrene co-acrylonitrile) of eight grades is studied to illustrate the approach. The design of single product plants is first investigated and the impact of the operating conditions on the different costs of the plant are discussed. Then, the design of a multiproduct plant with variable conversions in the polymerization reactors is performed. It was found that the incorporation of operating conditions in the design optimization allows higher utilization in time and capacity of the units, and increases the profitability by as much as 15% in our example.

ADMINISTRATIVE

The principal investigators has complied with the basic terms of the Agreement. Each of the investigators devoted 15% of time during the academic year and 33.3% of time during the summer to this project.

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