

Design Synthesis for Simultaneous Waste Source Reduction and Recycling Analysis in Batch Processes

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Abstract

The issues of waste generation in batch process plants differ in many aspects from those in continuous plants. Despite the smaller-scale of processing, complexities from discontinuities and run-to-run variations make waste minimization in batch plants more challenging. In this paper, we introduce an integrated qualitative-quantitative methodology and decision support system, called Batch-ENVOPE_{Expert}, for assessing waste minimization opportunities in batch processes. First, a qualitative analysis is performed to identify the sources of wastes and to derive recipe-level waste minimization solution. This is followed by detailed analysis at process variables level using mathematical simulation. The application of the methodology is illustrated using a propylene glycol case study.

Keywords: Waste Minimization; Expert system; Process improvement

1. Introduction

Batch process operations are prevalent in industries such as specialty chemicals, foods, agricultural chemicals, pharmaceuticals and other high value-added chemicals. Unfortunately, batch operations produce high waste-to-product ratio. In the past, batch process industries could tolerate large waste generation due to the high values of final products, which justify the waste treatment and disposal costs. However, due to increasing regulations, waste has become more expensive to deal with while market forces have constantly kept the product prices down. Today, this true cost of waste generation has provided a huge incentive for batch manufacturers to actively seek strategies for waste minimization.

Computer simulation has been applied to solve waste minimization problem through maximizing water reuse (Almato *et al*, 1999), recovering solvent (Lee and Malone, 2000) and minimizing environmental impacts (Jensen *et al*, 2003). One common shortcoming of the current simulation approach is due to the complexities involved in modelling industrial-scale process with large number of interconnections between the streams and units. Another shortcoming arises from the fact that this approach requires considerable skill and expertise of the user. We have previously addressed this important problem of industrial significance by developing a novel methodology for

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identifying waste minimization opportunities in continuous chemical processes (Halim and Srinivasan, 2002a). An intelligent decision support tool, called *ENVOPEExpert*, has also been implemented based on the methodology to automate waste minimization analysis in continuous plants (Halim and Srinivasan, 2002b, c). *ENVOPEExpert* has been successfully tested on several case studies including hydrocarbon separation process, chemical intermediate manufacturing, hydrodealkylation (HDA) of toluene to benzene and acrylic acid production.

In this paper, we extend the *ENVOPEExpert* methodology to batch processing environment. While the equipment used in batch process are readily available in continuous plant, the modes of operating them are significantly different. Unlike in a continuous plant, wherein each equipment is dedicated to one type of operation, the same equipment in batch plant is commonly used to perform multiple operations. These fundamental differences between batch and continuous operation necessitate new developments in the underlying knowledge representation and inference schemes that were implemented in *ENVOPEExpert*. In the next section, we discuss our proposed methodology called *Batch-ENVOPEExpert* and apply it to solve an industrial case study involving a propylene glycol process.

2. Waste Minimization Methodology of Batch Process

Our methodology has been developed with the following task: *given a flow diagram, production recipe and process chemistry of a batch process plant, the objective is to identify potential waste minimization alternatives*. For this, we implement a two-stage approach for source detection, diagnosis and waste analysis i.e. (1) Waste source tracing, and (2) Waste minimization options generation. In the first stage, the origin of each material component that makes up the waste stream is determined. As multiple operational tasks may be performed in the same piece of process unit, analysis of the production recipe thus plays a central role for identifying the waste generating operation. Once the waste sources are identified, the next stage is to derive waste minimization alternatives, i.e. source reduction or segregation and recycle of the useful materials for other purposes. This requires an integrated qualitative–qualitative methodology comprising Grafcet, process graph (P-graph) and mathematical modelling.

2.1 Grafcet model

Grafcet has been used for representing the production recipe of batch processes (Viswanathan *et al*, 1998). In our Grafcet model, each action in the product recipe is modelled using steps and the conditions associated with each action by transitions separating adjacent steps. Fig.1 shows a typical Grafcet representation. The recipe depicted in this figure describes a reaction-separation activity and can be explained as follows: (1) Two reactants (A and B) are charged into a vessel, (2) The vessel is heated to a specified temperature, (3) The mixture reacts to form product C and waste by-product D, and (4) The mixture is separated into product and waste stream.

2.2 P-graph model

We have used P-graph (Friedler *et al*, 1994) to describe the state condition of materials at the input and output of each process unit. Our P-graph takes a slightly different approach from the original P-graph, in which, a bar is used to represent an operation in the product recipe and a circle for state of materials of a unit operation or a stream. Fig.2 illustrates the P-graph representation for the recipe described in Fig.1. After the materials flow throughout the process has been established, the next step is to diagnose each operation that produces wastes as well as inefficient separation that causes the

escape of valuable materials into the waste streams. This is done by tracing each waste material backward, starting from each of the waste streams and upstream to the material flow network composing the product recipe. Fig.3 depicts the origins of waste stream shown in Fig.2. As shown in Fig.3a, the presence of product C in the waste stream is caused by inefficient separation process [Task 6]. The presence of by-product D, on the other hand, is caused by the reaction in the vessel [Task 4] (see Fig.3b).

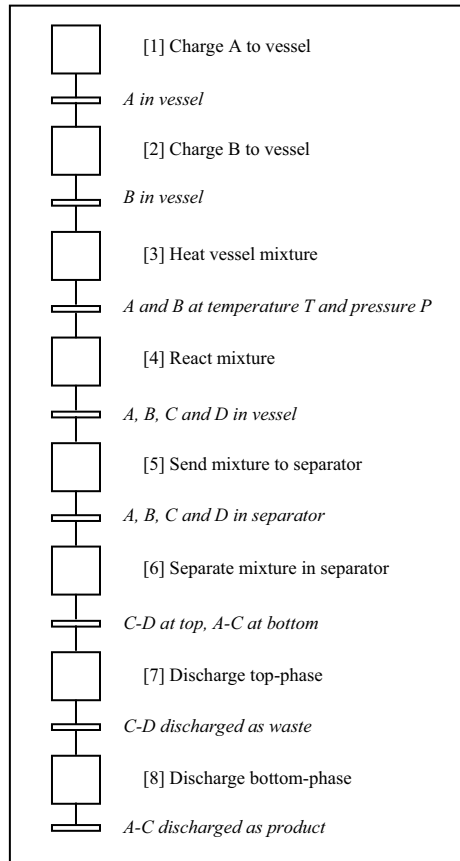


Figure 1. Grafcet of a product recipe

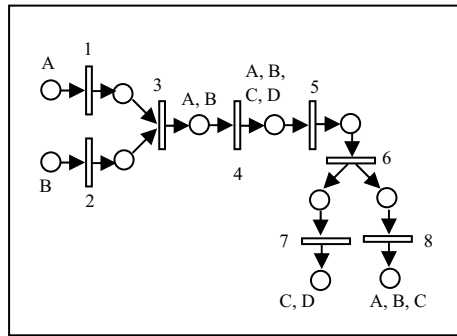


Figure 2. Material flow diagram

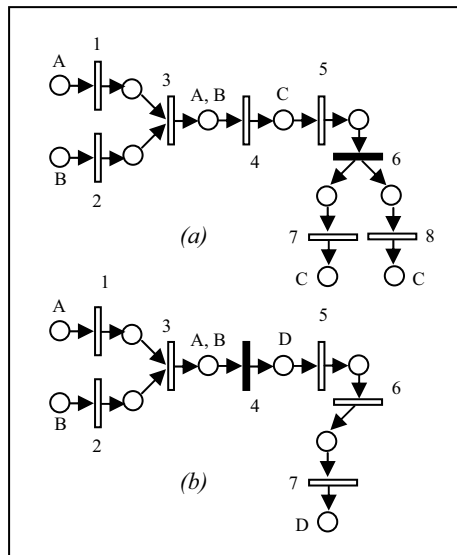


Figure 3. Waste flow diagram

2.3 Recipe-level waste minimization solution

Once the waste origins are identified, alternatives to eliminate or minimize them can be proposed. For this, we have derived a set of top-level waste minimization heuristics on the basis of P-graph analysis. These heuristics are implemented through IF-THEN rules set as the following:

- IF useless materials (e.g. impurities) are present in feed stream or feed equipment THEN remove those useless materials prior to usage.
- IF useful materials (e.g. reactants or products) are present in waste stream THEN recover and recycle those materials for other purpose.

- IF useless materials are generated during a reaction or other phenomena THEN eliminate or minimize the generation through better operating conditions.
- IF useful materials (e.g. reactants) are transformed at low conversion rate THEN increase the conversion rate for those materials.
- IF useful materials are ineffectively separated THEN improve the separation process to eliminate or minimize the escape of useful materials.

The heuristic approach provides a very top-level view of waste solutions. The next step in the quest for minimizing waste is to identify more detailed solutions at the process variable level that can be incorporated into the plant operations. The detailed analysis would provide suggestion on which process variables or parameters should be manipulated in order to achieve the desired waste reduction. To derive such detailed alternatives, cause-and-effect among the process variables need to be known and this can be obtained from signed digraph model or from mass and energy balance equations.

2.4 Detailed waste minimization solution

Signed digraph can be used to describe the cause-and-effect relation between two variables in a qualitative manner. It consists of nodes which represent process variables and directed arcs connecting the nodes to describe the relationship (“proportional” or “inversely-proportional”) between the nodes. The advantage of signed digraph model is it is simple to develop, especially when the availability of process data is limited. The main disadvantage is it cannot be used to describe variables with non-linear relationship such as variables with J-Curve relationship. Other disadvantage of signed digraph arises from ambiguities or incorrect relationship that may arise from multiple variables interaction. As an example, consider an output variable “flow”, which is connected to two input variables “pressure” and “heat-input” of “proportional” and “inversely-proportional” relationship respectively. Here, we will have ambiguity in describing the value for variable flow when both the input variables are increased. To avoid ambiguity, a more concise variables interaction model needs to be used. In our model, this is done using balance (mass and energy) equations.

We have developed sets of balance equations of several unit operations commonly found in a batch plant. Each unit operation model is directly linked to each activity in the product recipe that takes place in that unit. For example, the task of reaction in an agitated vessel can be modelled by mass and energy balances of stirred tank reactor, while the separation task will be represented by flash-separator, distillation column models, and so on, depending upon the type of separation unit utilized. To illustrate this concept more clearly, consider a waste minimization alternative “improve the reaction operating conditions to minimize waste by-products generation” that is derived using the P-graph model. Provided we have adequate process data, we can simulate the effects of different variables such as pressure, temperature and heat-input of the reaction to obtain the exact amount of waste being generated. This can be done through changing (either by increasing or decreasing) those affecting variables individually or simultaneously and comparing the results obtained in terms of the amount of waste produced and end product as well as economics. Consequently, process changes that cause waste to be reduced will be our waste solutions.

3. Intelligent Decision Support System

Batch-ENVOPE*Expert* (BEE) has been implemented in an object-oriented framework using Gensym's G2 expert system shell. BEE consists of two solutions domain: qualitative solution based on recipe analysis and quantitative solution based on

simulation of process variables. For the quantitative part, we have used HYSYS simulator as our modelling tool, although other commercial simulators could also be used. Fig.4 shows the overall framework of BEE. First, different stand-alone unit operation models are developed using HYSYS simulator. These models are then interfaced with Microsoft Excel through HYSYS-Browser program, which has been developed by AspenTech. The Excel program will consist of sets of input-output variables connected in two-way direction with their related unit operation in the HYSYS simulator. In this way, any changes to the input values in Excel will be passed to HYSYS for simulation and the results of calculation obtained will be transferred from HYSYS back to Excel. To link between G2 and Excel, an ActiveX based connection has also been developed in G2 system to interpret the simulation results on the basis of waste minimization and economic objectives.

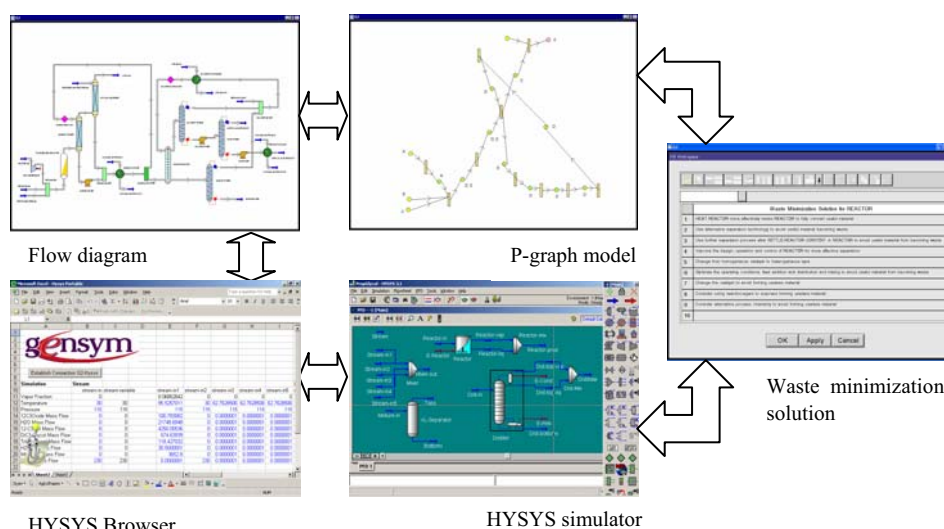


Figure 4. Batch-ENVOPE Expert Framework

4. Case Study: Propylene Glycol Process

We have tested our BEE by performing waste minimization analysis on a case study involving propylene glycol production (see Fig.5). The recipe for this process involves charging reactants (propylene-oxide and water) into a vessel in the presence of sulphuric acid as catalyst and methanol as the reaction aid. Besides (mono) propylene glycol product, the reaction also produces di- and tri-propylene glycol as the by-products. After a certain time, the reaction is quenched with sodium hydroxide solution before being sent to batch-distillation column for separation. The only waste stream of this process comes from vapour venting of the vessel and this stream contains mainly the excess reactants, methanol and mono- and di-glycol. For more detailed information on the production recipe and kinetics of this process, the reader is referred to Elgue *et al* (2003).

Our P-graph analysis for this case study reveals the following waste sources: reaction by-products and useful materials in the waste stream (vent). Based upon this diagnosis, the recipe-level and detailed waste minimization alternatives to the sources can then be derived. Table 1 shows some of the waste minimization results of BEE. In this case, we are able to successfully identify the basic qualitative and quantitative solutions.

However, the table also shows conflicting suggestions. Decreasing the pressure is found to reduce di-glycol in waste stream while increasing it can reduce propylene oxide from becoming waste. Such conflict is not uncommon in a waste minimization study, where trade-off between various options is always required for the most optimum solutions.

5. Conclusions

The issue of cleaner production has challenged the batch manufacturing industries to initiate new approaches to tackle waste problems. We have developed a methodology for automating identification of waste minimization strategies in batch processes and successfully implemented it as an intelligent system called *Batch-ENVOPEXpert*. The methodology has been shown capable in generating waste minimization solutions both in qualitative and quantitative manner. Our future work will include incorporating environmental impact and economic analysis into the current framework for trade-off analysis between the solutions.

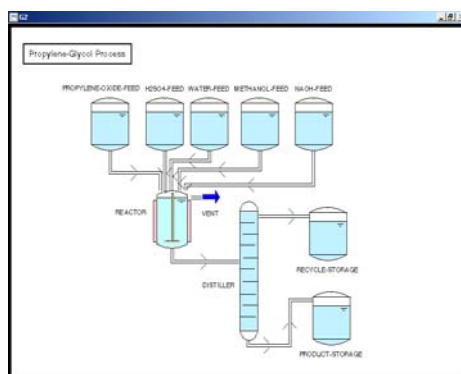


Figure 5. Propylene glycol process

Table 1. BEE solutions

Waste Minimization	
Qualitative	Direct-recycle or recovery-recycle of useful materials from vent. Improve the design and operation of vessel. Improve reaction condition. Change from homogeneous catalyst to heterogeneous one. Consider using reaction agents to suppress by-products formation.
Quantitative	Decrease 5% of feed pressure during reaction reduces di-glycol in waste stream from 574.6 kg/h to 567 kg/h. Increase 5% of feed pressure during reaction reduces propylene oxide in waste stream from 100.7 kg/h to 84.3 kg/h. Decrease 5% of feed temperature during reaction reduces di-glycol in waste stream by 574.6 kg/h to 572.5 kg/h.

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