A New Methodology for Automating Waste Minimization Analysis of Batch Processes

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ABSTRACT

The issues of waste generation in batch process plants differ in many aspects to continuous plants. Despite the smaller-scale of processing, complexities from unsteady state profiles, discontinuities, and run-to-run variations make waste minimization in batch plant more challenging. In this paper, we present a systematic methodology for waste minimization analysis of a batch process. The methodology consists of three fundamental elements: process graph (P graph) for process recipe assessment and path flow analysis of waste material and cause-and-effect and functional knowledge for evaluating the process recipe and equipment variables connectivity. The application of the methodology is illustrated through an alcohol washing case study.

1. INTRODUCTION

Manufacturing of chemicals through batch processing is dominant in industries such as specialty chemicals, foods, agricultural chemicals, consumer products, pharmaceuticals and other high value-added chemicals. Unfortunately, batch operations produce high amounts of waste per unit of product. As product quality and purity requirements need to be strictly controlled, multiple solvents and equipment cleaning agents are often excessively used, leaving a high volume of waste to be treated. In the past, batch process industries could tolerate high waste generation due to their high value of final products which outstrip the waste treatment and disposal costs. However, waste has become more expensive to deal with while market competition has kept the product price down. Today, this true cost of waste generation has provided a huge incentive for batch manufacturers to engage in waste minimization measures.

Despite its importance, waste minimization is still occasionally undertaken within the industries. One of the reasons is lack of specialized knowledge and technical expertise within the company that is crucial for successful implementation. To address this problem, we have previously developed a systematic methodology for automatic generation of waste minimization solutions (Halim and Srinivasan, 2002a). An intelligent decision support tool, called ENVOP*Expert*, has also been implemented based on the methodology (Halim and Srinivasan, 2002b, c). ENVOP*Expert* has been successfully tested on several continuous processes including a hydrocarbon separation, a chemical intermediate manufacturing process, a hydrodealkylation process of toluene to benzene and an acrylic acid production. In this paper, we extend ENVOP*Expert* methodology to batch processing environment. While the equipment used in batch process are readily available in continuous plant, the mode of utilizing them are significantly different. Unlike in continuous plant, in which each equipment is dedicated to one type of operation, the same equipment in batch process plant is commonly used to perform multiple operations. For example, a stirred jacket-heated vessel may be used to blend reactants, carry out a reaction, boil off solvent or distill the product. As results, various waste streams differing in composition, quantity and quality may be generated from the same piece of equipment during the operation. These fundamental differences between batch and continuous process operation necessitate new developments of the underlying knowledge representation and inference schemes that were implemented in ENVOP*Expert*. In the next section, we will describe our methodology in more detailed and apply it to solve an industrial case study involving an alcohol washing process.

2. WASTE MINIMIZATION METHODOLOGY

A waste can be defined as any material or energy input into a process that is not incorporated into the desired final product (Jacobs, 1991). If we trace the origin of each of the components in the waste stream, one or more of the following sources can be obtained: (1) unrecovered raw materials (2) unrecovered products (3) useful by-products (4) useless by-products (5) impurities in raw materials (6) spent process materials. Thus, finding waste minimization solutions for any process plant is in-fact equivalent to identifying the sources of each material component that make up the waste stream and finding ways to eliminate them. Our waste minimization methodology employs such a fundamental approach through a two-step procedure for waste analysis and diagnosis.

In our approach, each material that makes up a stream is classified as useful or useless by referencing it to its function in the overall process. Raw materials, solvents, cooling and heating agents, and products are the examples of useful materials, while material impurities and waste by-products fall under the category of useless material. A material should be considered useless only if it serves no useful purpose at all in the process. For example, hydrogen sulfide, a compound normally present in crude oil as impurity, should not be classified as useless if it is converted to saleable sulfur in a downstream process. In this case, such material is classified as useful raw material. Using this nomenclature, the following heuristic is thus deduced: *useful material cannot be produced from useless material*.

2.1. P Graph for Waste Flow Analysis

The first step in our methodology is to represent the flow of materials in each stream and process unit during the entire batch production. As multiple operational tasks may be performed in the same piece of equipment, the process recipe of batch process plays a central role in waste analysis. For this, we have adapted process graph (P-graph) to represent the state of material input and output in the process unit corresponding to each of the recipe tasks. Our P-graph model originates from the work of Friedler *et al* (1994) for representing process structure to solve the synthesis problem in a continuous process. In their P-graph, a material stream is represented by a circle, an operating unit by a bar and connections between material streams and operating units by directed arcs. Our P-graph takes a slightly different approach from the original P-graph, in which, a bar is used to represent an operational task in the process recipe and a circle for state of materials in a unit operation. To establish the presence materials in each stream and equipment for each recipe task, we employ qualitative simulation using information based on process flowsheet, material presents at each input stream, and the reaction, separation and phase change phenomena that take place over the predefined operating conditions. For example, a task of reacting material A and B in a reaction vessel at an operating condition which allows a reaction to takes place happen will be represented as an input node containing A and B and an output node of material A, B, C and D in the vessel.

To illustrate this application of P graph more clearly, consider an alcohol washing case study shown in Figure 1. This case study is taken from a waste minimization report by DuPont (1993) on one of its plants. A stream of crude specialty alcohol containing impurities enters a wash kettle and is mixed with washing agents comprising of water, chemical scavenging agents and isopropyl alcohol (IPA). The mixture is then heated, agitated and allowed to settle for few minutes. The washed alcohol separates from the washing agents and settles to the bottom of the kettle. The settled alcohol product is then drained and sent to an accumulator tank. When the alcohol product has drained and the aqueous wash has started to exit the kettle (as seen by the operator from the sight glass), the flow to the accumulator tank is diverted to a sump for wastewater disposal. Once the content inside the wash kettle is completely drained, the alcohol product from the accumulator tank is returned to the wash kettle for a second wash with the same washing agents. Again, the mixture is heated, agitated, allowed to settle and drained, with the specialty alcohol product going to the accumulator and the aqueous wash to the wastewater sump. From the accumulator tank, the specialty alcohol is then filtered and sold as final product.

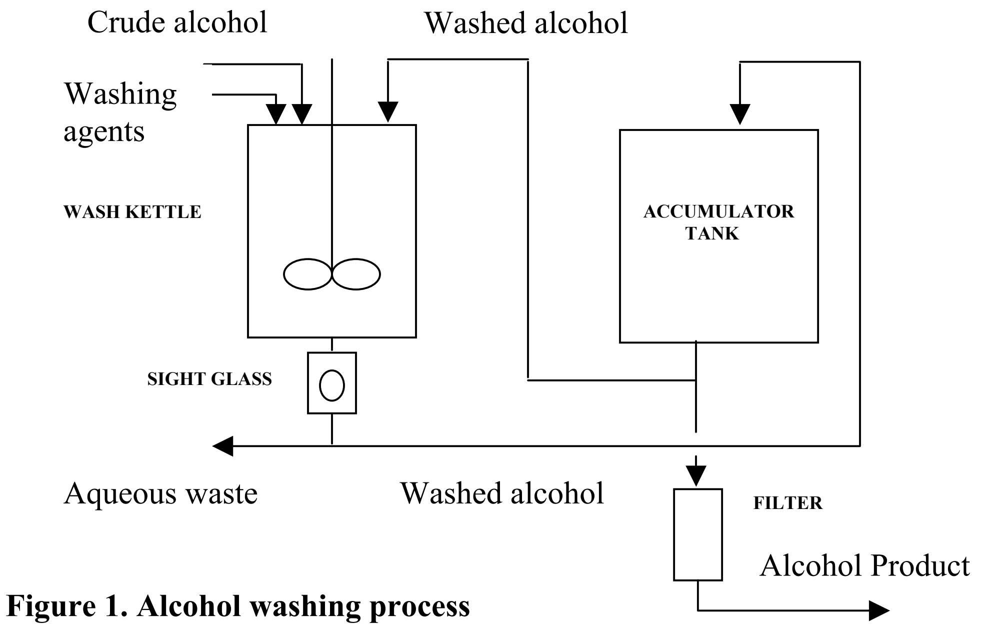


Figure 1. Alcohol washing process

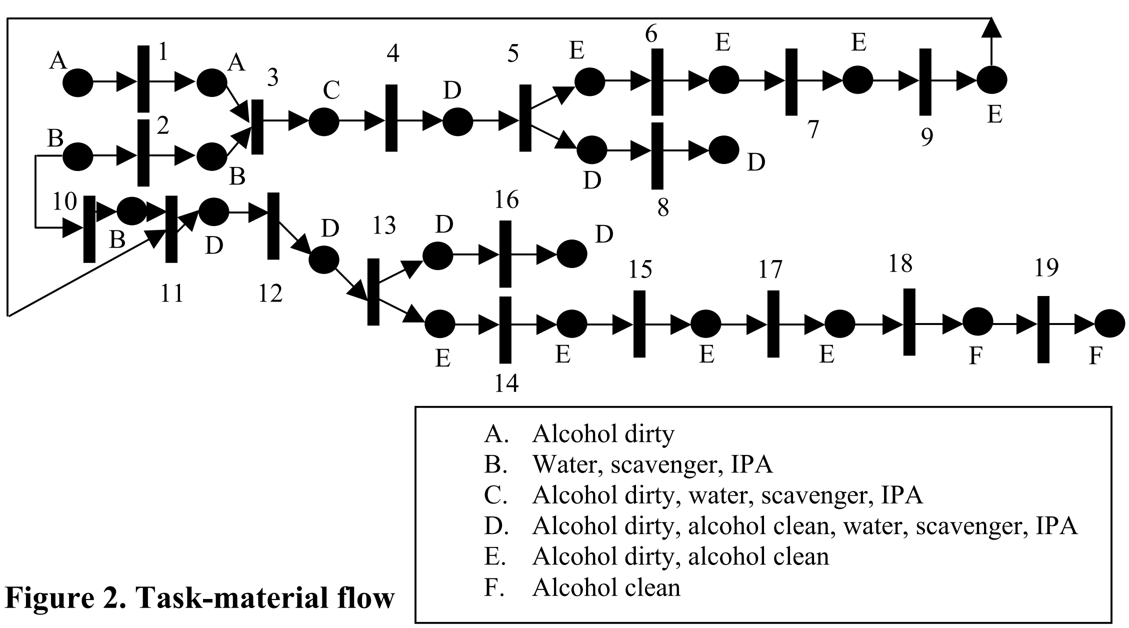


Figure 2. Task-material flow

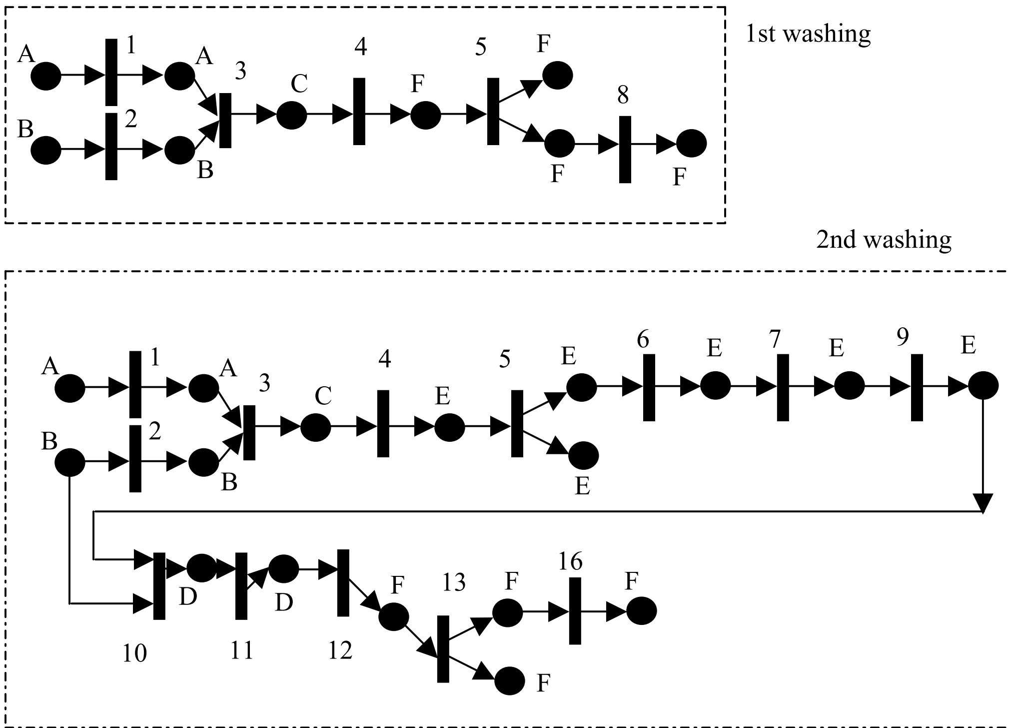
Figure 2 illustrates the P-graph representation of material flow for each of the tasks specified in Table 1. Starting with dirty alcohol (node A) and washing agents (node B), the series of operations performed (1-19) result in clean alcohol product (node F, subtask 19) and waste solution from first washing (node D, subtask 8) and second washing (node D, subtask 16). Once the flow of materials throughout the different unit operation of different operational task has been established, the next step is to diagnose the tasks and their related process units that contribute to the presence of each material in the waste streams.

For this we perform backward tracing of each waste material starting from the waste streams and upstream to the material flow network composing the recipe tasks, to establish the origins of each material component in their respective waste streams. Figure 3 gives the example of material flow of clean alcohol during the two washing. The presence of clean alcohol in the waste streams of the respective washing is mainly due to the following activities: (1) charging dirty alcohol (2) inefficiency in fully converting dirty alcohol to clean alcohol during the washing task (3) inefficiency in separating dirty alcohol and also clean alcohol during the settling operation. Once the waste origins are identified, alternatives to eliminate them can then be proposed as follows:

- Recycle useful materials in the waste stream
- Prevent excessive charging of dirty alcohol into the washing vessel
- Improve settling operation to segregate clean alcohol from becoming waste stream (subtask 5 and 13)
- Improve conversion of dirty alcohol to clean alcohol in the washing vessel (subtask 4 and 12)

Table 1: Process recipe for alcohol washing process

Task Name	Subtask Description	Subtask Code
First washing in kettle	Charge vessel with crude alcohol	1
	Charge vessel with washing agents	2
	Heat vessel content	3
	Agitate vessel content	4
	Settle vessel content	5
	Transfer bottom layer to accumulator tank	6
	Store bottom layer at accumulator tank	7
	Transfer top layer to sump	8
Second washing in kettle	Charge vessel with alcohol from accumulator tank	9
	Charge vessel with washing agents	10
	Heat vessel content	11
	Agitate vessel content	12
	Settle vessel content	13
	Transfer bottom layer to accumulator tank	14
	Store bottom layer at accumulator tank	15
	Transfer top layer to sump	16
	Transfer content of accumulator tank to filter	17
Filter product	Filter alcohol mixture	18
	Transfer filtrate product	19



A. Alcohol dirty
B. Water, scavenger, IPA
C. Alcohol dirty, water, scavenger, IPA
D. Alcohol dirty, alcohol clean, water, scavenger, IPA
E. Alcohol dirty, alcohol clean
F. Alcohol clean

Figure 3. Waste flow of clean-alcohol washing process

The above mentioned waste minimization alternatives provide a very top-level view of 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 variables and the function of the unit operation need to be known.

2.2. Causal Relationship for Variables Interaction

We have adapted digraphs to describe physico-chemical phenomena that possibly take place inside relevant unit operations during the task (or subtask) action. In our approach, phenomena and affecting variables associated with each task are represented as nodes connected with directed arcs. Each node can take values "increase" or "decrease" and the directed arcs can take the values "+" to describe proportional or "-" for inversely proportional relationship between two nodes. As an example, consider the simple cause-and-effect model of a washing task shown in Figure 4. We have modeled this washing task as a reaction process in which dirty alcohol is converted into clean alcohol. In this case, the conversion of dirty alcohol is influenced directly by processing time and reaction coefficient which is also affected by reaction time and agitation speed. Through this digraph representation, the alternative “improve the conversion of dirty alcohol to clean alcohol in the washing vessel” from the P graph analysis can be translated as: “increase washing time”, “increase washing temperature” and “increase agitation speed”.

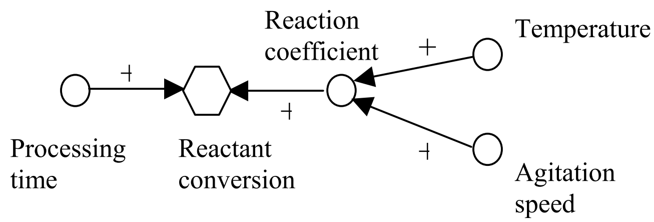


Figure 4. Digraph of clean-alcohol washing process

2.3. Task Connection Using Functional Modeling

The objective of functional modeling is to facilitate interactions between the different tasks performed in the process. In our approach, the functional knowledge of each task is associated with main variables that are directly influenced by that task action. For example, temperature is the main variable for a cooling or heating task while stirring-speed is for agitation task. Consider the waste minimization alternative “increase washing temperature” which is derived using digraph model. This alternative is closely in line with the task of “heating the mixture in the vessel” since temperature is the main variable of this task. In this case, the alternative “increase washing temperature” can be further elaborated as “increase the temperature during heating of the mixture”. In the same manner, the alternative “increase agitation speed” can be further described as “increase the stirrer speed during agitation”. Thus, for a given batch process plant that comprises sets of interconnecting streams and unit operations, different variables of the interacting tasks in the process operation can be linked together to support the overall waste minimization goal.

3. COMPARISON

We have performed a waste minimization analysis using our systematic methodology on the alcohol washing process and compared the results of our analysis with the available waste minimization team’s solutions. Table 2 presents this comparison between the team’s findings with the ones obtained using our methodology. As shown in the table, we are able to successfully identify more waste minimization alternatives than the team by following the systematic methodology.

4. CONCLUSION

Waste minimization is one of the most important issues facing the batch chemical industry today. In this paper, we describe a systematic methodology for waste minimization analysis for any batch chemical process plant. The methodology consists of heuristic rules and methods, which diagnose the sources of wastes using P-graphs and recommend top-level waste minimization which can be defined in more detailed using cause-and-effect digraphs and functional models. The comparison between the waste minimization options generated by our methodology and by a team of experts shows that our methodology is able to accurately identify basic waste minimization solutions. Currently we are developing an automated system based on this methodology and implement it to solve more complex case studies.

Table 2. Comparison of waste minimization team's results and our methodology

Team's results	Our methodology
Wash alcohol once instead of twice	Perform the washing process once only
Recycle second wash to first wash of next batch	Recycle second or after waste stream for the next process
Replace washing process with acid neutralization process Employ alternative chemistry to eliminate acid residual in waste stream	Use alternative separation technology Use further separation action after settling operation in washing vessel
Vacuum-strip IPA from waste stream for recycling	Direct-recycle or recovery-recycle of the useful material in waste stream
Substitute a less toxic solvent for IPA Use salt solution instead of IPA	Substitute IPA with others material
Wash alcohol at higher temperature	Increase the temperature during heating of the mixture Increase the agitation speed during agitate mixture Increase the process time during agitate mixture
	Improve the design and control of washing vessel
	Install larger accumulator tank to facilitate better separation in washing vessel

REFERENCES:

E.I. Du Pont de Nemours, DuPont Chamber Works Waste Minimization Project, November 1993

Halim, I.; Srinivasan, R. Systematic Waste Minimization in Chemical Processes: Part I. Methodology. *Industrial Engineering and Chemistry Research* **2002**, 41(2), 196

Halim, I.; Srinivasan, R. Systematic Waste Minimization in Chemical Processes: Part II. Intelligent Decision Support System. *Industrial Engineering and Chemistry Research* **2002**, 41(2), 208

Halim, I.; Srinivasan, R. An Integrated Decision Support System for Waste Minimization Analysis in Chemical Processes. *Environmental Science and Technology* **2002,** 36(7), 1640

Friedler, F.; Varga, J.B.; Fan, L.T. Algorithmic Approach to the Integration of Total Flowsheet Synthesis and Waste Minimization. In *Pollution Prevention via Process and Product Modifications*; American Institute of Chemical Engineers: New York, 1994.

Jacobs, R.A. Waste Minimization–Part 2: Design Your Process for Waste Minimization. *Chemical Engineering Progress* **1991**, 87(6), 55.