# Designing Waste Minimization Alternatives for Batch Processes Using an Intelligent Simulation-Optimization Framework

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## Abstract

The issue of environmental sustainability has prompted the batch chemical industries to switch from end-of-pipe treatment to waste minimization as top priority in tackling the pollution problem. In this paper, we introduce a novel simulation-optimization framework that integrates different process systems engineering (PSE) methodologies – process graph (P-graph), hierarchical design strategy, WAR algorithm, source-sink allocation method, and multi-objective optimization as decision making tools for waste minimization analysis. The framework is applied to a well-known literature case study and yields convincing results.

*Keywords:* sustainable development, intelligent system, process synthesis, multi-objective decision making, simulated annealing

## 1. Introduction

Batch processing has been the preferred operating mode in the manufacturing of high-value added chemicals such as pharmaceuticals, fine and specialty chemicals, and agrochemicals. In contrast to bulk chemicals that are produced using continuous processes, the demands for high-value chemicals are seasonal and low in volume. In this regard, batch operation with its intrinsic operational flexibility is the most appropriate to use. However, compared to continuous process, batch process exhibits a more challenging problem. While the size of batch plants is generally smaller than their continuous counterparts, batch manufacturing typically generates high waste per unit of production. In fine chemicals and pharmaceutical processes, for example, it is fairly common to generate 100 kilogram of wastes per kilogram of product (Sheldon, 1997). In the mean time, the time-dependent characteristic of batch process present difficulties for effective waste recovery as the intermitten flows of streams from different parts of the process pose contraints to optimal reuse or recycle of the streams. With the current drive towards eco-sustainability (as exemplified by Kyoto Protocol), the batch chemical producers are now facing mounting pressure to minimize their emissions, as well as raw-material and energy usages. All these factors have motivated us in developing a framework – one that is robust and efficient for evaluating design alternatives for waste minimization opportunities in the batch plants.

Given the complex and multidisciplinary nature of waste minimization analysis, a systematic way of identifying suitable design alternatives is thus essential. Previously, we have developed BATCH-ENVOP*Expert* – an intelligent system that derive and evaluate qualitative alternatives to sources of waste as well as inefficient operations in the process (Halim and Srinivasan, 2006). In this paper, we introduce an advanced BATCH-ENVOP*Expert* version that amalgamates three domains: knowldege-base approach, process simulation, and mathematical optimization for more comprehensive and cost-effective waste minimization analysis. We illustrate this framework by testing it on a well-known literature batch operation case study involving reaction and distillation (von Watzdorf *et al*., 1994).

## 2. Waste Minimization Framework

The statement for waste synthesis problem of a batch plant can be defined as the following: *Given the equipment flowsheet, operating procedure (production recipe), and process chemistry of a plant, identify potential waste minimization alternatives and propose process changes which simultaneously reduce the environmental impact and improve the profit*. To answer this challenge, we have developed an advanced BATCH-ENVOP*Expert* framework that integrates different process systems engineering (PSE) methodologies in a robust manner. Figure 1 shows the architecture of the framework, which is modeled after the procedures of conducting a waste minimization study to a process plant. Overall, it involves the following elements:

- waste source diagnosis through material component tracking,
- rule-based qualitative waste solutions and identification of process variables underlying the waste features,
- quantification of environmental and economic performances through indicators,
- stochastic optimization to identify region of optimal plant performances.

Each of these elements has been successfully implented using different methodologies which are described next.

### 2.1. Qualitative Waste Minimization Analysis

To track the sources of waste in the process, we have implemented process graph (P-graph) approach. P-graph originates from the work of Friedler *et al*. (1994) who demonstrated a special directed bipartite graph for representing process structure suitable for the synthesis problem. In the P-graph model, 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. Using P-graph, all streams and unit operation that contribute to the presence of each different material component in each process waste stream can be traced. The reader is referred to Halim and Srinivasan (2002, 2006) for detailed description of P-graph model. In general, there are five sources that can be identified through P-graph analysis:

- useless material in inlet stream,
- excessive feed of useful material in inlet stream,
- useful material transformed at low conversion rate,
- useless material produced from reaction or phase change phenomena, and
- ineffective separation of useful material.

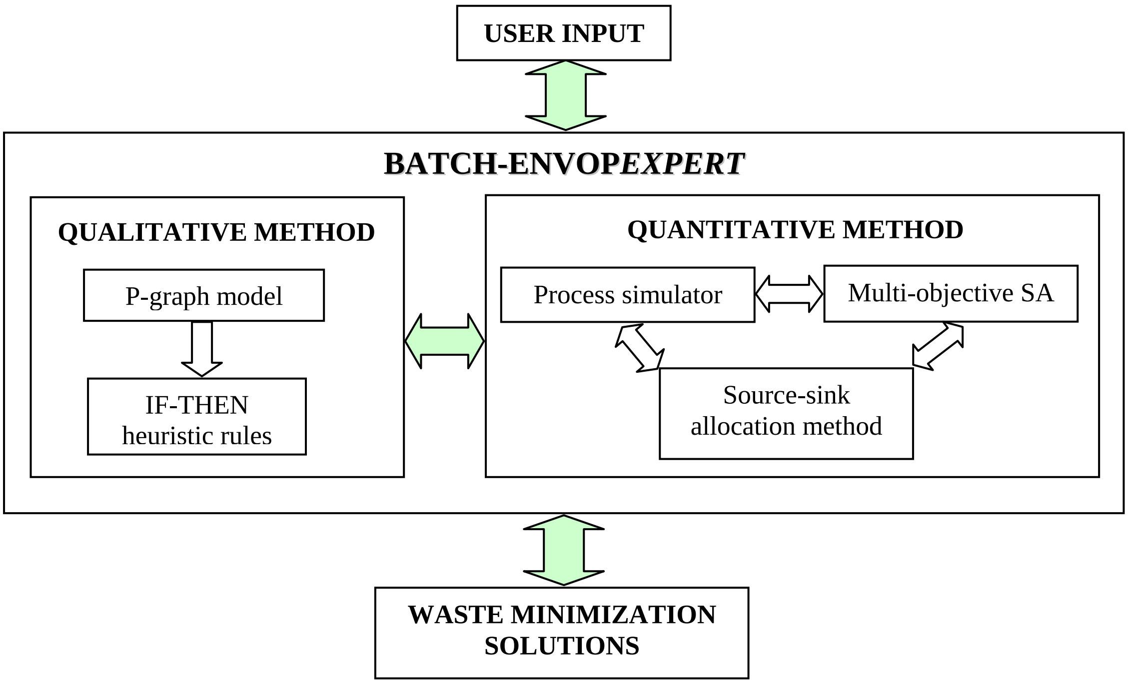


**Figure 1. BATCH-ENVOP*Expert* Framework**

Once the waste sources are diagnosed, hierarchical design approach are applied to derive solutions to those sources. These heuristics, which analyze the P-graph to locate the high-level modification required in the process, are in-line with the sets of IF-THEN axioms approach by Douglas (1992) and Smith (1995) and can be summarized as follows:

- Reduce useless materials in the material feed
- Reduce waste byproducts formation
- Improve the reaction and phase change operations
- Improve the separation operation by adding an extra separation unit
- Recovery and recycle of the useful material from waste stream

While heuristic suggestions provide potential modifications, their efficacy to the plant can be justified when reduction in the waste amount can be demonstrated. Apart from qualitative alternatives, the inference algorithm of P-graph is also capable of deducing which variables to be accounted for to reduce the waste generation. This is done by representing each of the waste generating phenomena by the main process variables affecting the phenomena. For example, consider the P-graph suggestion “optimize the reactor condition to eliminate waste-byproduct”, their main variables – temperature, pressure, and flow of the reactants can be modified to alter the reaction outcomes. This is performed in the next stage of analysis.

### 2.1. Simulation-Optimization Approach

We have combined the process simulation approach with WAR environmental impact (Cabezas *et al*., 1999) and cost impact calculations. However, like many other design problems, the environmental impacts and economic aspects of the proposed alternatives may conflict one another. For example, increasing the reactant flowrate to reduce the byproducts formation would lead to higher operating costs. To resolve these conflicts, we use a heuristic search algorithm, simulated annealing, to identify design strategies that satisfy the multiple objectives.

We have implemented simulation-optimization framework as a tool for variable modifications. The term “simulation” implies the use of simulator for simulating the output of the process plant in response to changes in the input variables. We have used gPROMS dynamic simulator for this purpose although other commercial simulators may also be applied. The term “optimization” signifies the application of mathematical optimization algorithm to find the most optimum variable settings to improve the objective functions that are not defined by explicit mathematical equations but a simulation model. We have adapted the multi-objective simulated annealing framework of Suppapitnarm *et al*. (2000) to find an entire set of Pareto-optimal solutions. In general, the framework involves the following iterative procedures:

- Randomly generate a solution vector $X$, whose elements are the process variables that control the waste generation profile.
- Simulate the batch process using the new variables to derive a vector of objective function $Y$.
- Evaluate each element of these new objective functions by comparing it with the one stored in the Pareto set and update the set using the nondominated criteria.
- For non-archived solution (dominated vector), calculate the probability function P and compare it with a randomly generated probability function $P_{rand}$. When $P > P_{rand}$, vector X is retained.

### 2.3. Source-Sink Mapping Methodology

One of the high-level modifications that is highlighted by BATCH-ENVOP*Expert* is reuse (recycle) of waste streams for other purposes. We have implemented a source-sink allocation method (El-Halwagi, 2006) for developing optimum recycle network. The method can be expressed as follows: *Given a plant with its set of process sinks, process sources that can be recycled to the sinks, and fresh resources that supplement the flow of process sources, create a network of connections between them with objective of minimum flow fresh resources subject to pre-specified flowrate and* *composition constraints*. Figure 2 illustrates this methodology. In our approach, process sources represent the waste streams that can be recycled to other operations. Example is the recycling of waste water from the first operation to the second, etc. Fresh resources, in this context, are the fresh water that is originally used in the washing process. Thus, by maximizing the flow from sources to sinks, the fresh water usage and concomitantly the waste water discharge can be minimized.

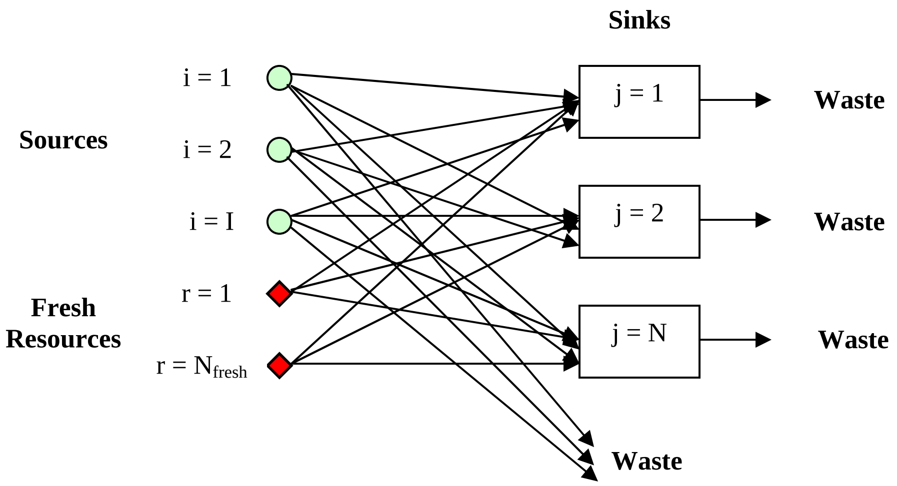


**Figure 2. Source-Sink Allocation Problem**

The following equation expresses the objective function of minimizing the total flow of fresh resources ($F_r$):

$$Min \sum_{r=1}^{N_{fresh}} F_r \qquad (1)$$

A mass balance constraint of the process sources that can be assigned to the various process sinks and wastes can be described as:

$$W_i = \sum_{j=1}^{N_{sink}} w_{i,j} + w_{i,waste}\text{, where } i = 1, 2, \ldots, N_{Source} \text{ and w is the stream flow} \qquad (2)$$

Similar constraints to the total fresh resources and total wastes can be written as:

$$F_r = \sum_{j=1}^{N_{sink}} f_{r,j}\text{, where } r = 1, 2, \ldots, N_{fresh} \qquad (3)$$

$$\text{Total waste} = \sum_{i=1}^{N_{source}} w_{i,waste} \qquad (4)$$

On the other hand, the mass and concentration balances over mixing of streams entering the process sinks are expressed as:

$$G_j = \sum_{i=1}^{N_{source}} w_{i,j} + \sum_{r=1}^{N_{fresh}} f_{r,j}\text{, where } j = 1, 2, \ldots, N_{sink} \qquad (5)$$

$$G_j \times z_j^{in} = \sum_{i=1}^{N_{source}} w_{i,j} \times y_i + \sum_{r=1}^{N_{fresh}} f_{r,j} \times x_r\text{, where } j = 1, 2, \ldots, N_{sink} \qquad (6)$$

while the concentration bounds of the stream entering the sink is defined as

$$z_j^{\min} \le z_j^{in} \le z_j^{\max} \quad \text{where } j = 1, 2, \ldots, N_{sink} \qquad (7)$$

The resulting mathematical formulation is of linear programming type and can be solved for global optimum using GAMS.

## 3. Application to case study

We have applied the framework using a case study shown in Figure 3. The process starts with reaction between chemical A and B in a jacketed vessel to produce product C and byproduct D. The reaction process is performed three cycle and involves filling the vessel with reactant A followed by adding a small flow of B. As the reaction is exothermic, once the temperature reaches a certain level, cooling of the reactor is started to maintain a constant temperature. The reaction is then allowed to proceed until the yield of product C reaches its maximum value. At that point, the reactor is cooled with the maximum cooling capacity to rapidly bring the temperature to the ambient level. The reaction mixture are transferred to an intermediate storage tank and the reactor vessel washed with cleaning liquid. From the storage, the mixture is transferred to a vessel and batch distilled to produce two main cuts of high purity A and C. The final residue from distillation is byproduct D, which is then sent to a separate storage. In this process, two waste streams are generated: spent cleaning liquid and waste-byproduct D. Our objective here is to derive waste minimization alternatives pertinent to these waste streams.

Table 1 shows the proposed qualitative solutions for this process. In the next stage of analysis, optimization is performed using simulated annealing technique to minimize the environmental impact, batch cycle time as well as maximize the product throughputs. In this case study, the following variables are set as the decision variables – cooler set point, reboiler set points at different stages of operation, and purity specifications of A and C. Simultaneously, a source-sink allocation method is implemented to minimize the use of cleaning liquid through recycling. Table 2 shows the optimization results. Compared to the base case design operation, maximum improvement of 8.1%, 0.7%, and 3.8% can be observed for the product flow, batch time, and environmental impact objective, respectively. Also, a 63.7% reduction in the cleaning liquid waste is obtained through recycling alternative.

## 4. Conclusions

Waste minimization is an important element in green process engineering. We propose integrating the knowledge-base approach with process simulator and mathematical optimization technique to derive comprehensive and cost-effective waste minimization solutions. Through this, we can capitalize on the complementary perspectives – heuristic methods and rules from the knowledge-base system, modeling and simulation capabilities of the process simulator, and stochastic optimization capabilities of simulated annealing. The framework has been tested using a literature case study. The results clearly show the capability of BATCH-ENVOP*Expert* as an intelligent “clean design” decision support system.

**Table 1. Qualitative waste minimization alternatives**

| Stream/Unit | Waste minimization solution |
|---|---|
| T103 | Substitute cleaning liquid with other material<br>Prevent excessive use of cleaning liquid |
| R101 | Consider alternative process chemistry or use reaction agent to surpress forming useless byproduct<br>Optimize the reaction condition to eliminate byproduct and fully convert material A |
| T105 | Reuse or recycle of cleaning liquid waste<br>Recycle the liquid waste to the next cleaning process |
| T110 | Reuse or recycle of waste byproduct stream |
| T106 | Use alternative separation technology to avoid useful material from becoming waste<br>Use further separation after the vaporization process to void useful material from becoming waste<br>Improve the separation condition |

**Table 2. Pareto-optimal solution**

| Status | Product flow | Batch time | Environmental impact | Cleaning liquid flow |
|---|---|---|---|---|
| Base case | 2839.5 | 12937 | 1238.4 | 3228.4 |
| Pareto set | 3011.8 | 12864 | 1205.1 | 1203.3 |
| | 2922.7 | 12848 | 1219.2 | 1201.4 |
| | 3063.7 | 12842 | 1193.3 | 1205.9 |
| | 3053.4 | 12909 | 1199.5 | 1203.4 |
| | 3064.5 | 12915 | 1195.7 | 1207.1 |
| | 3090.1 | 12918 | 1191.3 | 1208.8 |

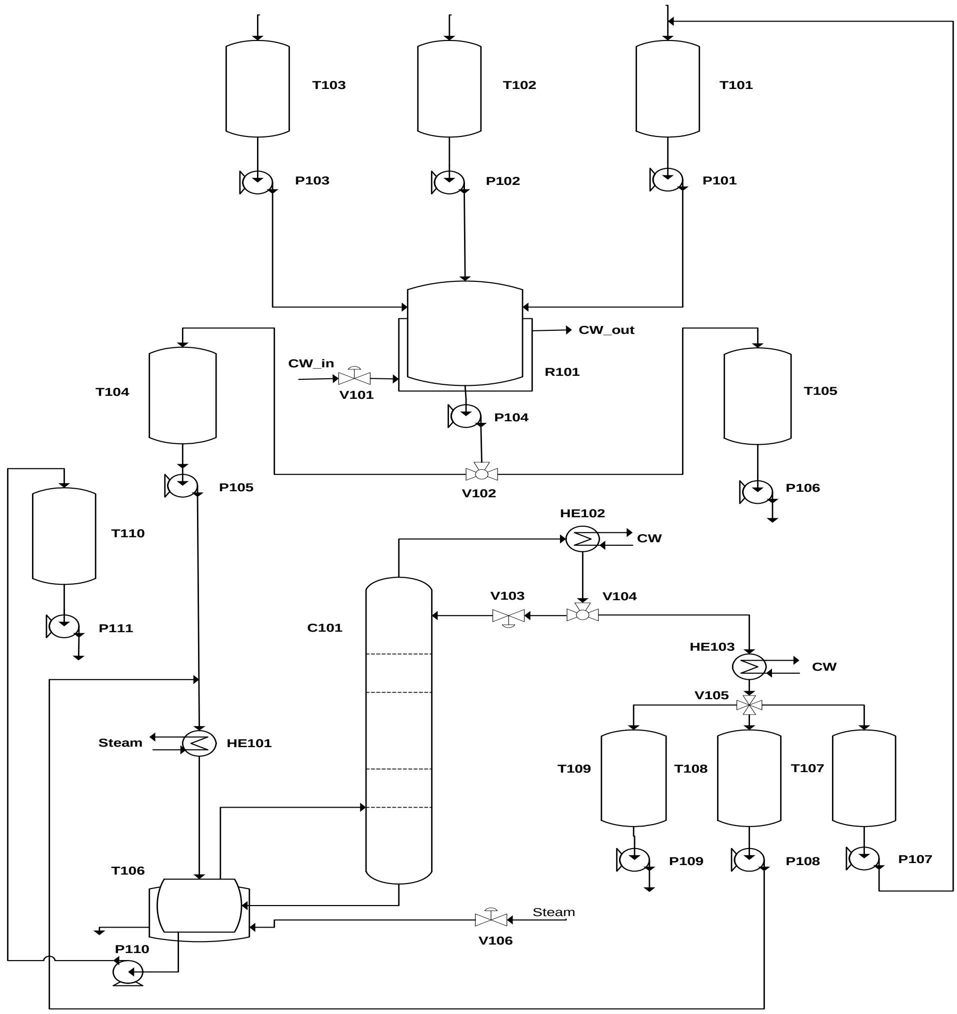


**Figure 2. Batch Process Case Study**

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