Systematic Waste Minimization in Chemical Processes. 1. Methodology

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Increasing public pressure, more stringent regulations, and escalating waste treatment and disposal costs have motivated the chemical industries to implement waste minimization at the source rather than to rely on end-of-pipe treatment. Waste minimization analysis is time-consuming, expensive, laborious, and knowledge-intensive. The objectives of this two-part paper are (1) to develop a systematic methodology to guide a nonexpert with the technical aspects of waste minimization and (2) to implement an intelligent system that can automatically perform a waste minimization analysis of a chemical process plant. In part 1, a systematic methodology for waste minimization analysis is presented. An intelligent decision support system that implements this methodology is presented in part 2. The proposed methodology comprises three fundamental elements: process graph (P graph) and cause-and-effect and functional knowledge. The P graph is a directed bipartite graph capable of abstracting the flow of materials in a process. An analysis based on the P graph provides a framework for diagnosing the origins of waste in the process and for deriving top-level waste minimization alternatives. These top-level alternatives can then be distilled further by using cause-and-effect and functional knowledge to obtain detailed alternatives. The application of the methodology is illustrated using an industrial case study.

1. Introduction

In a chemical process, the transformation of raw materials into useful products is accompanied by the generation of waste. Apart from creating potential hazards and environmental problems, wastes also represent a loss of valuable materials and energy from the production units. Billions of dollars are spent annually by chemical facilities worldwide to meet the discharge standards imposed by local authority. Traditionally, pollution prevention has been achieved through treatment processes added at the end of the production line. However, this end-of-pipe treatment approach is no longer viewed as adequate, because it does not actually eliminate waste but simply transfers it from one medium (air, water, or land) to another. For example, the removal of a toxic compound from a gas using an aqueous solvent in a gas−liquid contactor would necessitate the treatment of the resulting "contaminated" aqueous stream before it is discharged to the receiving water body. Further treatment of the aqueous stream would generate precipitated sludge, which at the end would require safe landfill disposal. Increasing public awareness of the impact of industrial pollution, more stringent discharge standards, and escalating waste treatment and disposal costs have put enormous pressures on the chemical industries to shift their paradigm of pollution prevention from the end-of-pipe treatment to waste minimization or even total elimination at the point of generation.

In the United States, the Environmental Protection Agency (EPA) has declared waste minimization as the top-priority action in the waste management hierarchy.[1] Waste minimization primarily involves two main principles: source reduction and recycling (see Figure 1). Source reduction includes changing the product through substitution or composition changes and controlling the waste at the source through input material changes, technology changes, and good operating practices. On-site and off-site recycling activities include direct use or reuse of the waste in the same or another process and waste reclamation for other useful purposes. When implemented, the benefits from the waste minimization activity are vast, encompassing various facets of the company, and include[2] (1) economic benefits through cost savings in waste treatment and disposal, reduced raw material, energy, and utility usage, and increased process productivity and reliability, (2) health and safety benefits, by reducing the risk associated with handling hazardous materials, (3) legal benefits, by reducing the risk of breaching environmental regulations and the resulting liabilities, and (4) benefits from an improved public image.

Despite the many benefits, systematic waste minimization in chemical plants is only occasionally undertaken, and even then in a small scale because of several issues perceived to hinder the successful implementation of a waste minimization program. Although reducing waste quantities brings down waste compliance costs and increases production revenue, the initial cost of implementing a waste minimization program is a significant economic deterrent. Unreceptive response and resistance to change among different elements may also discourage the progress of the program. However, the most important reason, which is commonly cited for waste minimization studies to be considered a high-risk activity, is the lack of specialized knowledge and techni-

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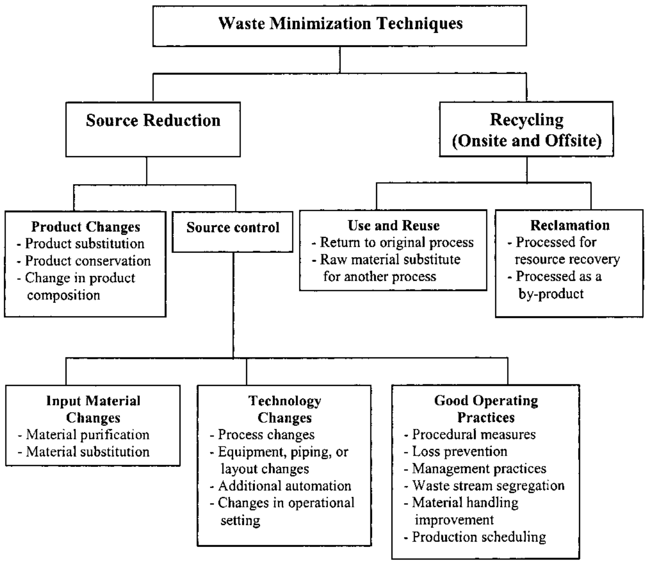


Figure 1. Outline of waste minimization techniques.

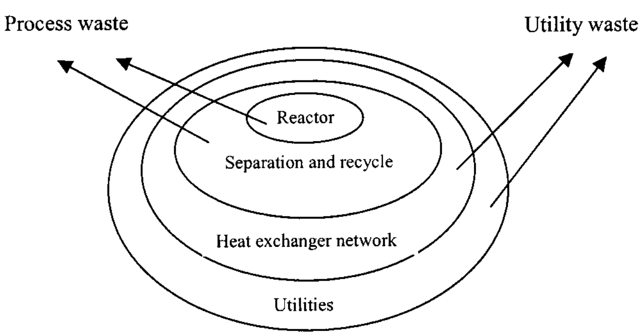


Figure 2. Onion diagram of waste generation origins.

cal expertise within the company that is crucial for successful implementation.

Research in the area of waste minimization has resulted in numerous techniques and methodologies to be published in the literature. In the broadest sense, all of these available techniques can be classified into quantitative and qualitative approaches. The quantitative approach to waste minimization is basically through the application of pinch technology or numerical optimization for solving the synthesis problem of heat- and mass-exchange networks of the process in concern. Pinch technology has been widely used in the process industry to save energy via improvements in the design of heat-exchange networks (HEN).[3] This is achieved by reducing the overall energy consumption through better heat integration between the hot and cold streams of the process. Consequently, the environmental benefit becomes apparent through the reduction of fuel-combustion-related emissions such as NO_x, SO_x, CO_x, and particulates. El-Halwagi[4] extended the principles of HEN to material wastes by introducing the concept of a mass-exchange network (MEN), a technique for the optimal design of a mass-transfer operation network. The synthesis problem of MEN can be defined as follows: given a number of waste streams and a number of mass-separating agents (MSAs), such as solvents, adsorbents, stripping agents, and so forth, synthesize an MEN that can preferentially transfer certain undesirable species from the waste streams to the MSAs at minimum cost. To solve this problem, the MEN synthesis is formulated as a numerical optimization problem

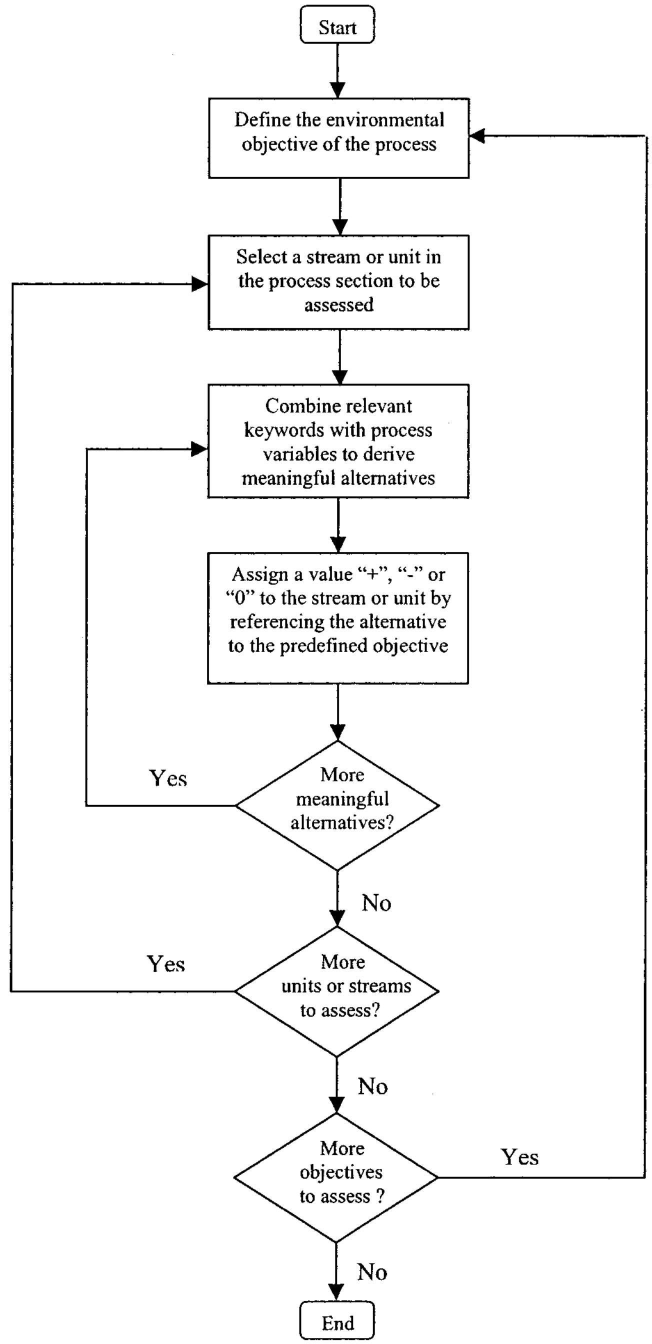


Figure 3. ENVOP sequential procedure.

subject to thermodynamic, mass-transfer driving force, and economic constraints.

In the qualitative approach, methods such as the Douglas hierarchical procedure, onion diagram, 3Es methodology, and environmental optimization are used to identify the possible waste minimization alternatives for the process. In Douglas' procedure,[5] the hierarchical decision structure for process design as developed by Douglas[6] is extended to incorporate potential strategies to reduce waste generation right from the early stages of design. The basic waste minimization solutions that can be derived through this procedure can be summed up as changing the chemistry, changing the process, changing the equipment, changing the solvent, and reusing and recycling the material. Smith[7] reported another hierarchical approach based on the onion diagram, where waste arising from the process is

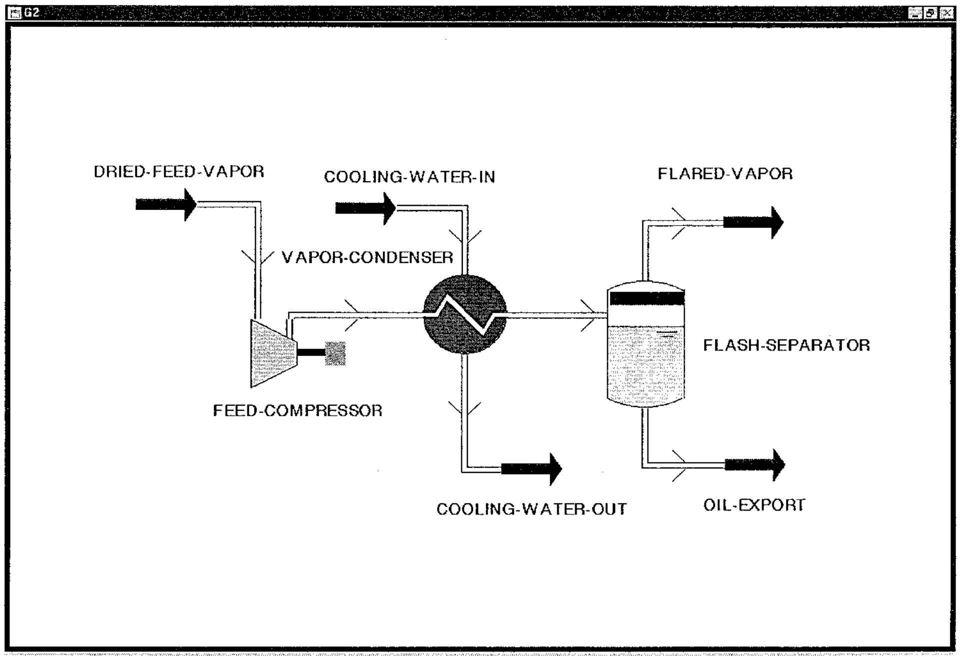


Figure 4. Downstream section of the hydrocarbon separation process.

categorized into two classes by relating its origin to a layer of the onion diagram (see Figure 2). The two inner layers, which correspond to the activities of the reactor and separation systems, generate process waste, while the outer layers, which define the HEN and utility system, produce utility wastes. In this procedure, the quest for waste minimization follows the steps of process synthesis, starting from the innermost layer (reactor design) and moving to each subsequent outer layer. The 3Es methodology is a technique developed by Her Majesty's Inspectorate of Pollution (HMIP) in the United Kingdom for identifying potential environmental improvements of a process.[8] The procedure involves creating a series of "what if" scenarios for different elements of the process, including materials, unit equipment, employees, and procedures. The scenarios focus on three factors: reduced emissions, improved efficiency, and economic benefits. Some examples of the what if scenarios that may result are the following: what are the implications to the environment and production when (1) alternative raw materials are used, (2) control equipment is installed in a reactor unit, or (3) production scheduling is implemented into the process? Once feasible scenarios are found, they are then implemented to improve the performance of the process.

1.1. ENVOP Technique. Another qualitative approach to waste minimization is environmental optimization (ENVOP), a technique jointly developed by Costain Oil, Gas and Process Ltd. and BP International.[9] The sequence of a typical ENVOP analysis is shown in Figure 3. The procedures behind the ENVOP technique are similar to the ones in a hazard and operability (HAZOP) analysis commonly used for process safety and the 3Es methodology. During an ENVOP study, a team of experts systematically evaluates each line and equipment of the process to identify potential waste minimization alternatives that meet environmental objectives such as (1) reduction of vapor and liquid emissions, (2) reduction of solid waste sent to a landfill, (3) savings in utility consumption, and so forth.

The team identifies meaningful alternatives by combining a set of qualitative guidewords (such as more, less, etc.) with process variables (such as pressure, temperature, flow rate, etc). Table 1 lists some process variables and guidewords commonly used in an ENVOP study. Each alternative is assessed by referencing it to the predefined environmental objectives; a value of "+" is assigned to an alternative that meets the objective, a "−" if it violates the objective, and a "0" when no relation is found between the alternative and the corresponding objective. This procedure is repeated for different streams and units of the process to generate as many alternatives as possible, each of which is then analyzed on the basis of technical and economical feasibilities.

Table 1. Process Variables and Deviation Guidewords Used in ENVOP

variable	guidewords
flow	no, more, less, recycle/bypass
temperature	more, less
pressure	more, less
level	more, less
composition	change, add, remove, phases
stream/equipment	more/larger, less/smaller, alternative

The following case study illustrates the application of the ENVOP procedure to a real-life industrial waste minimization problem. This case study involves the downstream compression−flash separation section of a hydrocarbon separation process first described by Isalski.[9] Figure 4 shows the basic flow sheet of the process. An incoming vapor stream containing a mixture of hydrocarbons (C1 to C5) is initially compressed to high pressure in the feed compressor followed by condensation using cooling water in a heat exchanger. The resulting vapor−liquid mixture is flashed in a separator from which the liquid from the bottom is used as product. The vapor from the top is a waste and is sent to a flare system. An ENVOP review can be carried out for this process with the objective of reducing the hydrocarbon vapor sent to the flare system. Several alternatives can be identified as shown in Table 2 of which "less hydrocarbon feed to the process", "more flow rate of cooling water", and "add glycol coolant to the cooling water stream" are feasible and would be further analyzed for implementation. For a comprehensive

Table 2. ENVOP Review of a Hydrocarbon Separation Process

guideword	variable	alternative	reduction of vapor
less	hydrocarbon flow rate	less hydrocarbon feed	+
no	cooling water flow rate	no cooling water	−
more	cooling water flow rate	more cooling water	+
less	cooling water pressure	less pressure of cooling water	0
add	cooling water stream	add glycol to cooling water	+
recycle	vapor stream	recycle vapor to condenser	0
larger	flash separator	larger size of flash separator	0

review of the ENVOP procedure, the reader is referred to work by Isalski.[9]

While the ENVOP technique provides an overall structure for conducting a waste minimization analysis, it does not provide a technique for resolving contradicting suggestions. For example, in the previous case study, the alternative "add glycol coolant to the cooling water stream", while effective in minimizing the hydrocarbon emissions, would generate environmental impact elsewhere during the blowdown process. In addition, it does not provide any detailed guidance on how to identify the source of waste and the changes that can be made to the process to eliminate them. It is, therefore, difficult for a nonexpert to apply ENVOP, especially for large-scale processes. It is, thus, highly desirable to develop a more structured methodology to guide the nonexpert during a waste minimization analysis. Such a methodology must be capable of identifying waste sources that arise in the process, assisting the nonexpert in terms of possible suggestions that eliminate or minimize the waste sources, and highlighting the environmentally friendly suggestions which result in the least environmental impact. Another requirement for the waste minimization methodology is that it should be amenable to automation. We address these important problems in this paper by developing a systematic methodology, broadly based on the ENVOP technique, that can be used to detect and diagnose wastes in a process and also help to identify alternatives to eliminate or minimize them. In part 2, we develop an expert system that uses this systematic methodology for automating a waste minimization analysis.

2. Intelligent Approaches to Waste Minimization

Despite its importance, the development of intelligent systems for automating a waste minimization analysis has been limited. Most of the previous work is from the perspective of process operations and is process-specific. Only a few have addressed the problem from the perspective of design and synthesis. Huang and Fan[10] developed a hybrid intelligent system using a knowledge base augmented with fuzzy logic and neural networks to design an optimum HEN or MEN. In their approach, waste minimization is accomplished when the degree of structural controllability between the networks of interconnecting streams reaches a maximum and when the occurrence of undesirable disturbance propagation and their severities can be tolerated. This approach thus emphasizes quantitative waste minimization analysis from the perspective of process operation. Luo and Huang[11] developed an intelligent decision support system combining a knowledge base with fuzzy logic to help the plant operator identify waste minimization opportunities through process modifications and operational changes. However, their prototype is specific to electroplating processes. Research on automating waste minimization analysis for any chemical process from the perspective of process design was reported by Pennington,[12] who developed a set of design heuristics for several process units using mainly IF−THEN rules and embedded them into the prototype P2TCP expert system. In his system, options for minimizing waste generation and energy consumption were generated qualitatively through the physicochemical properties of the materials used and the reaction schematic occurring in the process, with no consideration given to the complex interactions between the different unit operations and streams of the process.

In this two-part paper, we propose a systematic methodology to guide the nonexpert with the technical aspects of waste minimization from the perspective of process design. This methodology is applicable to the various stages in the life of the plant, from conceptual design to process retrofitting. In part 1 of this paper, the waste minimization methodology is described and illustrated using a case study from the literature. In part 2, an intelligent system that uses this methodology to perform waste minimization with its application on a complex industrial case study is illustrated. The organization of the rest of this paper is as follows: In section 3, the proposed waste minimization methodology is introduced. In section 4, its application to a hydrocarbon separation case study is illustrated with results.

3. Methodology for a Waste Minimization Study

In a chemical process plant, the overall transformation of raw materials and energy into desired products is generally accompanied by the generation of wastes. Waste can be defined as any material or energy input into a process that is not incorporated into the desired final product.[13] In the context of a chemical process plant, wastes can be classified as utility waste and process waste.[7] In this paper, we focus on process wastes. The origin of each material component in the process waste stream can always be traced back to one or more of the following sources: (1) unrecovered raw materials, (2) unrecovered products, (3) useful byproducts, (4) useless byproducts, (5) impurities in the raw materials, and (6) spent process materials.

Therefore, finding waste minimization solutions for any process plant is equivalent to identifying the sources of each material component that make up the waste stream and finding ways to eliminate them. In this section, we present a waste minimization methodology which employs such an approach through a two-step procedure for source detection, diagnosis, and waste analysis.

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 byproducts fall under the category of

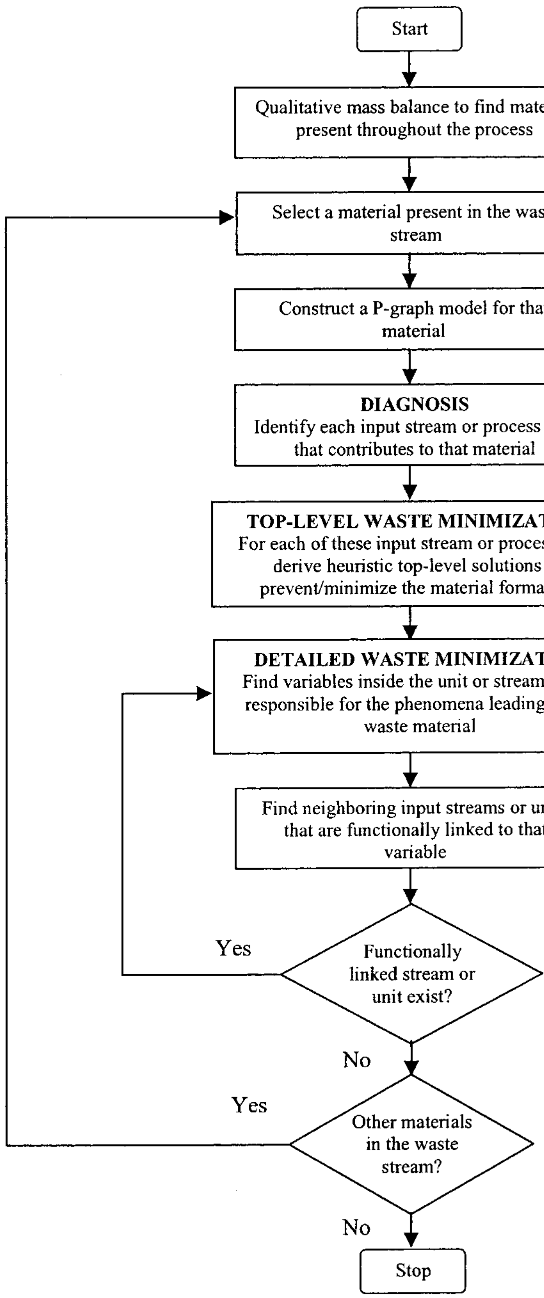


Figure 5. Systematic waste minimization methodology.

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 an impurity, should not be classified as useless if it is converted to saleable sulfur in a downstream process. In this example, our recommendation is that such material be classified as a useful raw material. Using this nomenclature, the following heuristics can be deduced: (1) useful material cannot be produced from useless material, and (2) useful material can produce either useful or useless material.

Figure 5 shows the sequence of steps employed in our proposed methodology. First, all of the materials present in each stream and unit of the process are determined. Because the composition of each material in a stream is not necessary, this can be easily performed for an operating plant on the basis of process knowledge and by using relevant drawings and available online and laboratory measurements. Alternatively, it can be easily

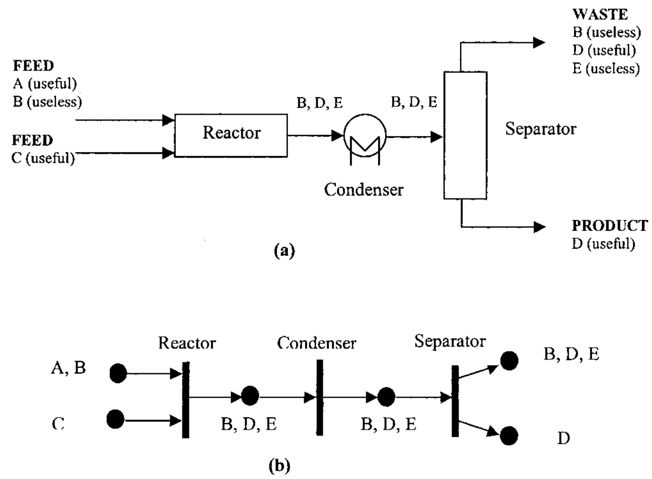


Figure 6. (a) Simple reaction−separation process. (b) P graph model for the process in part a.

obtained when a steady-state or dynamic simulation of the process is available. However, in the case of plants in the early stages of design, neither of these may be available. In such cases, the materials in each stream would have to be explicitly determined. This can be done using a qualitative simulation of the process flow if information about the process flow sheet, material present at each input stream, and the reaction, separation, and phase-change schemes that take place over the predefined operating conditions is available.

Once the materials present in the different parts of the process are established, the next step is to diagnose the streams and units that contribute to the presence of useful and useless material in the waste streams. Waste minimization alternatives would then aim to segregate the useful material from the waste stream and route it to product streams. Similarly, useless materials could be reduced at the source. These are achieved in our approach using a process graph (P graph) and cause-and-effect and functional knowledge.

3.1. Waste Source Identification Using a P Graph. The P graph originates from the work of Friedler et al.,[14] who demonstrated a special directed bipartite graph for representing a 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. Figure 6b illustrates the P graph model for the reaction−separation process shown in Figure 6a. In this process, two inlet streams, one containing raw material A with impurity B and the other containing raw material C, are fed to a reactor forming product D at a 100% conversion rate of the reactants A and C. Waste E is a byproduct of this reaction and impurity B an inert product. The reaction is followed by condensation and separation between B, D, and E. A P graph model is used to represent all streams and equipment that contribute to the presence of each different material component (whether useful or useless) in each process waste stream. This P graph representation of the process can be used for identifying the sources of waste and for generating waste minimization alternatives.

We have derived a set of top-level waste minimization heuristics on the basis of P graph analysis. In general, there are four sources of process waste: (1) useless material in an inlet stream, (2) useful material trans-

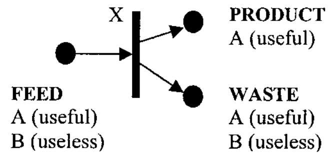


Figure 7. P graph of a simple separation process.

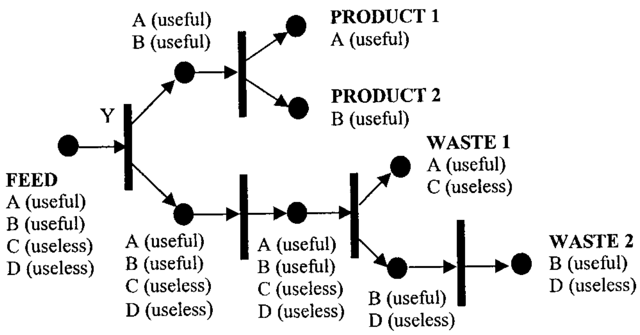


Figure 8. P graph of a complex separation network.

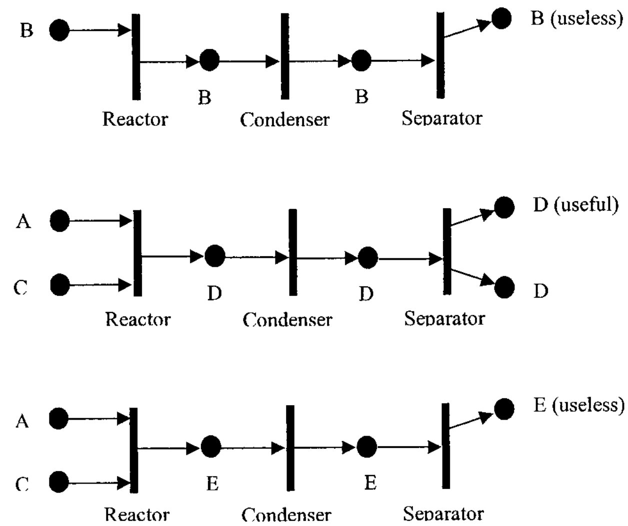


Figure 9. P graphs of materials in a waste stream.

formed at a low conversion rate, (3) useless material produced from reaction or a phase-change phenomena, and (4) ineffective separation of useful material.

Useless materials (impurities) that enter with the feed in the inlet stream will inevitably lead to waste.[7] To reduce feed impurities, alternatives such as removing or reducing those impurities from the inlet stream using a feed purification system or upgrading the quality of the raw material can be implemented. Useful material in the inlet stream may become waste when it is in excess or is transformed at low conversion rates and not adequately recovered. The solution for this involves preventing excessive feed of such material, increasing its conversion rate, or using direct recycling or recovery recycling of it from the waste stream back to the corresponding process unit. For reactor units that produce useless material, waste minimization involves changing the type or configuration of the reactor and optimizing the reactor operating conditions to eliminate or reduce the generation of waste material.

Inefficiencies in separation processes can lead to the escape of useful raw materials or products to the waste stream. We introduce the term “critical unit” to describe such separation units where inefficient separation between useful and useless materials leads to the presence of useful material in waste streams. To illustrate such a unit, consider the P graph model of a separation process shown in Figure 7. The unit X in Figure 7 inefficiently separates useful material A, leading to its presence in the waste stream. Unit X is thus a critical separator. Similarly, Figure 8 shows the P graph model for a complex separation network, where unit Y is not effective in separating useful materials A and B from the useless materials C and D and is therefore critical. Waste minimization alternatives corresponding to critical separators include adding an extra separation unit after the critical unit to increase the recovery of useful material or optimizing the design and operating variables affecting separation in the critical unit.

To illustrate the P graph approach for diagnosing waste sources, consider the process shown in Figure 6a. The objective is to minimize the waste stream, which contains three materials: B, D, and E. Figure 9 shows the P graph for each of these materials in the waste stream. Three sources of waste can be identified. Material B occurs in the waste stream because it enters the process as an impurity in the inlet stream. Product D occurs in the waste stream because of inefficient separation. Material E is formed as a byproduct in the reactor. Once the sources of waste are identified, alternatives for waste minimization can be proposed. In this example, alternatives include removing impurity B from the inlet stream, increasing the efficiency of the separator to prevent product D from leaving in the top stream, and optimizing the reaction between A and C to eliminate the production of byproduct E. Overall, an analysis based on the P graph model can thus be used to identify such top-level waste minimization alternatives for the process.

While the top-level alternatives act as a good guide to the specific waste minimization problem and provide potential solutions, the next step in the quest for minimizing waste is to identify detailed suggestions at the process variable level that can be incorporated into plant design and operations. The detailed analysis would provide suggestions on which process variables or parameters should be manipulated in order to achieve the desired waste reduction. Analysis based on the P graph model is not, however, capable of specifically determining the process variables in a process unit which are to be manipulated to reduce waste generation. To derive such detailed alternatives, the cause and effect among the variables and the function of the process unit need to be known.

3.2. Waste Minimization Option Identification Using Cause-and-Effect Knowledge. Cause and effect among the variables in a plant is usually a part of the mental model of plant personnel and design engineers. Such information can be systematically captured and represented using directed graphs (digraphs). Digraphs have been used for representing cause and effect in a chemical process system, especially in the field of fault detection and diagnosis. In digraph modeling, each process variable of the process units is represented as a node, and interaction between two variables is captured as a directed edge. Process variable nodes can take the values of high, low, or zero, and the arcs connecting the nodes can have the values directly positive (+) or negative (−), indicating the direction of influence of one variable deviation on another. Digraphs of various chemical engineering unit operations have been developed for automating HAZOP analysis.[15−17]

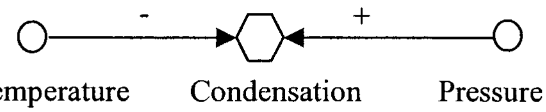
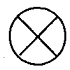
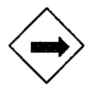
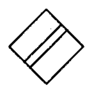
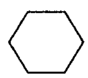
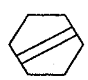


Figure 10. Digraph model of a vapor condenser.

Table 3. Basic Mass Flow Function Representation

Mass Flow Function	Symbol
Source	
Sink	
Transport	
Barrier	
Storage	
Balance	
Separate	

We have adapted digraphs to represent the cause-and-effect knowledge of process units required for waste minimization analysis. In our approach, process variable nodes can take the values' "increase" or "decrease", and the directed arcs can take the values' "+" to describe proportional or "−" to describe inversely proportional relationships between two nodes. We have also introduced a special node in our digraphs to represent physicochemical phenomena that occur in a process unit and are instrumental in waste generation. Examples of such phenomena are reactions producing waste byproduct and physical phenomena involving boiling, condensation, stripping, and absorption of materials. Any of these may lead to the presence of useful material in waste streams. In the digraph representation, these phenomena nodes are connected to different variable nodes that influence the phenomena. Through this, each variable corresponding to the "waste-generating" phenomena in a process unit can be identified and manipulated. As an example, consider the simple cause-and-effect model of a vapor condenser shown in Figure 10. The digraph has circular nodes denoting the process variables, an octagonal digraph node representing the vapor condensation phenomenon, and arcs connecting the temperature and pressure nodes to the phenomenon node. The reader would note that, as compared to the digraph models which have been previously reported in the literature, the cause-and-effect models required for waste minimization are simpler. This is because, in the waste minimization digraph models, only phenomena that are practically important from the waste generation perspective have to be represented and connected to variables responsible for the phenomena. Thus, while it is possible for the condenser unit to operate at zero efficiency (i.e., no condensation taking place), such a situation has no significance in generating waste, because it does not involve material being transformed or generated and does not have to be considered during waste minimization analysis.

Consider again the reaction−separation model as shown in Figure 6a. P graph analysis on material D reveals the low conversion (condensation) of D vapor in the vapor condenser as a waste-generating mechanism and suggests the top-level alternative "increase the condensation rate". This suggestion from the P graph analysis is transmitted to a condenser digraph through rules that conclude that the value's increase in the condensation digraph node. Subsequent propagation in the condenser digraph would use the values of the connecting arcs to infer that the pressure and temperature in the condenser should increase and decrease, respectively. This results in the detailed waste minimization alternative to "decrease temperature and increase temperature in condenser to minimize D in the waste stream". We have developed waste minimization digraph models of common chemical engineering process units, such as heat exchangers, absorption columns, distillation columns, compressors, pumps, and so forth, on the basis of material and energy balances and design heuristics.

In real life, the alternatives "increase the condenser pressure" and "decrease condenser temperature" will be achieved through changes in the units and streams upstream of the condenser. To identify such alternatives, one possible solution is to create a cause-and-effect model of the whole process by joining together the individual models corresponding to each stream and process unit. However, one major disadvantage of this approach is that combining individual models together to form a cause-and-effect representation of the overall process may lead to ambiguities or incorrect model behavior of the process.[18] This is due to multiple paths between pairs of nodes and, hence, multiple paths of influence between the nodes. In our approach, we propose using the function-centered knowledge (functional models) originally proposed by Modarres[19] to establish connections between different cause-and-effect models and avoid the problem of multiple causal paths.

3.3. Waste Minimization Option Identification Using Functional Knowledge. Functional modeling is an approach used to model any man-made system by identifying the designer's overall goal for a unit and the functions it must perform to fulfill the goal. Unlike classical modeling methods that explain the behavior of the physical structure of the system, functional models look at a system on the basis of its goal, function, and behavior. Functional models have been used in numerous areas including fault diagnosis[20] and design of industrial control systems.[21] While there have been several types of functional models proposed in the literature, our work is based on the multilevel flow modeling (MFM) approach proposed by Lind.[22] In MFM, the functional structure of a system is described using a set of interrelated structures for mass, energy, and

Table 4. Functional Models for Common Process Units

Units	Symbol	Functional Primitives	Functional Variables
Reactor	⊙	Generate Consume	Composition Temperature
Separator	▯	Separate	Composition
Compressor	◇	Generate Control	Pressure
Pump	◇	Generate Transfer	Pressure Composition
Condenser	⬡	Generate Maintain	Composition Temperature
Valve	◇	Generate Transfer	Pressure Composition
Storage tank	⬡	Maintain	Level

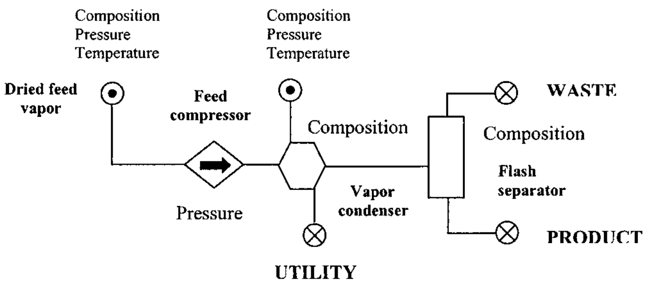


Figure 11. Functional model of a compression–separation section.

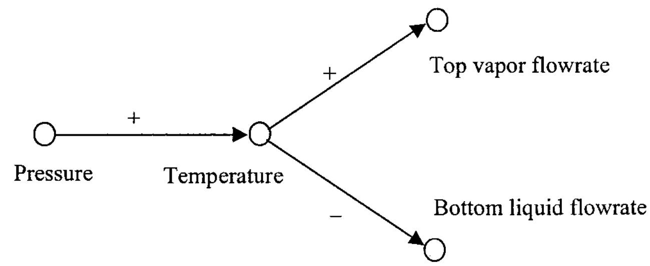


Figure 12. Digraph model of a flash separator.

information flows. These flow structures are built using the different flow types of source, sink, transport, barrier, storage, and balance as shown in Table 3. The interested reader is referred to Lind[22] for a detailed description of MFM and its applications.

We have adapted MFM for the alternatives-generation stage of waste minimization analysis. Because this work primarily focuses on material wastes, the mass flow structure of the process is sufficient for the analysis and is the only one considered here. In our approach, the functional knowledge of each unit is used to facilitate modeling of a process unit's interactions with its neighboring units and streams. From a waste generation point of view, each process unit and stream is considered to serve one or more functions out of a small set, including generate, consume, separate, control, transfer, and maintain.

As an example, consider a reactor where the reaction $A + B \rightarrow C$ occurs. This reactor can be considered a source of the reaction product C and a sink of reactants A and B; hence, its function is to "generate" C and "consume" A and B. Similarly, a distillation column can be considered to serve the "separate" function between the distillates and the bottoms. To integrate the functional models with the cause-and-effect digraph models discussed previously, we have linked the functions of the process units to the variables through which the the function expresses.

All of the variables cannot be directly manipulated in every process unit. For example, while temperature can be directly manipulated in a cooler by manipulating the coolant flow rate, temperature changes cannot be directly achieved in a pump. To achieve a lower temperature at a pump, we would need to seek a unit that is a source or sink of heat upstream of the pump, that is, a unit where temperature is a functional variable, and manipulate the temperature at that unit. Considering the reactor functional model as an example, through the generation of the reaction products and the consumption of the reactants, the variables that are directly influenced in the reactor are composition and temperature. Such variables are called functional variables. Similarly, pressure is considered the functional variable for a compressor and temperature for a cooler or heater. Functional variables are used to identify the process units that directly influence key variables in a section of the plant. The typical functions of common chemical engineering process units and their functional variables are shown in Table 4. The functional model of an entire process can then be synthesized by suitably combining the functional models of the process units in the flow sheet. As an illustration, the reader is referred to Figure 11, which shows the functional model of the process shown in Figure 4.

The overall waste minimization goal can only be realized if each stream and unit (systems) in the plant exhibits "clean" functions, such as no impurities in feed streams, no waste byproduct generation in reactors, and efficient separations. Such functions can only be achieved when each element of the system behaves to support such functions. The main role of functional models in our approach is to identify possible interactions between a unit or stream and its neighboring units and streams. When these functional interactions are established, different variables of the interacting units in the process can be linked together to support the overall waste minimization goal. On the basis of their functional variables, different units throughout the process that

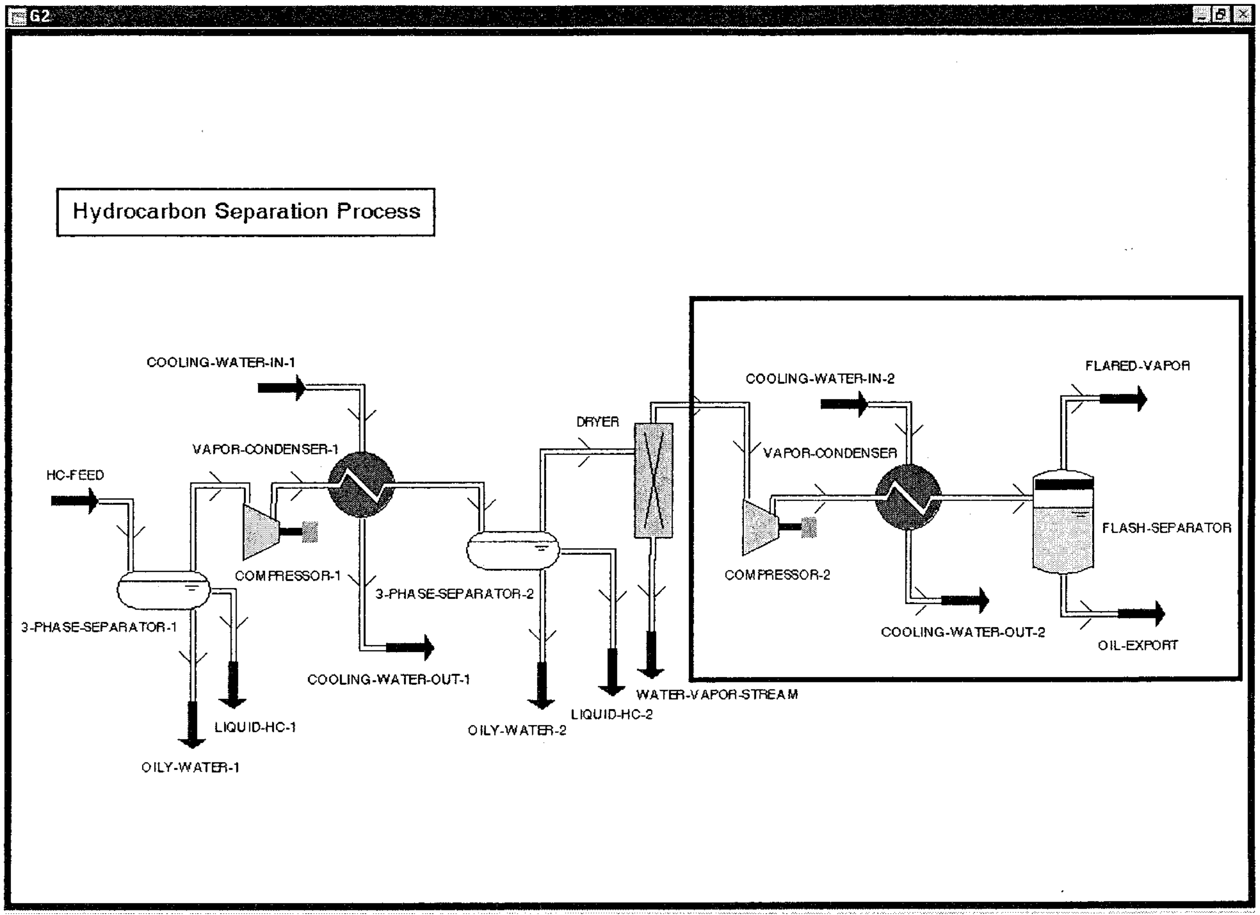


Figure 13. Hydrocarbon separation process.

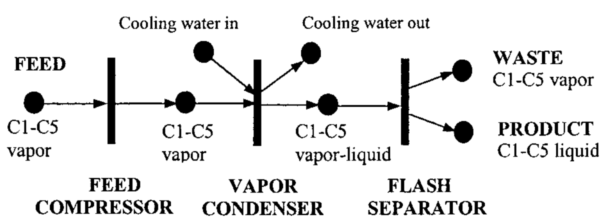


Figure 14. P graph representation of a compression−separation section.

share the same variables can be internally connected. Consequently, the cause-and-effect knowledge representation among the units that have the same functional variables can be linked together.

During alternatives identification, once it has been determined from the digraph model that a variable, say temperature, in a unit (U_x) has to be manipulated to minimize waste, we then search for other process units (U_y) in the neighborhood that have temperature as the functional variable. We can then look at the digraph model of U_y and identify its variables and the changes needed to achieve the necessary change in U_x. Similarly, if the phenomena node of that digraph model U_y demands that the pressure has to be changed, we then search for other units U_z downstream of U_y and identify the necessary changes in the relevant variables of U_z. To illustrate this role of functional modeling in bridging different digraph models and their connections with phenomena nodes, consider the example of a condenser connected upstream of a separator as shown in Figure 6a. Assume that the separator is a flash separator and that the reaction in the reactor is exothermic. The separator's cause-and-effect knowledge (Figure 12) establishes that the pressure and temperature directly affect the flow rate of the useful material D leaving from the top of the separator as waste. During the digraph analysis, this will be led to the alternative "decrease the top-vapor flow rate in separator", and the value "decrease" will be concluded for the top-vapor flow rate digraph node. All of the other nodes connected to it will be subsequently activated, indicating that the temperature in the separator has to be decreased. Because the temperature has to be manipulated, the process unit that has temperature as its functional variable (reactor) will be sought, and the suggestion "decrease temperature in reactor" will be synthesized to support the waste minimization objective. In this manner, given a process flow sheet with interconnected streams and units, the entire chain of functional interactions in the flow sheet can be established.

4. Case Study: Hydrocarbon Separation Process

To illustrate the proposed methodology, consider the hydrocarbon separation process shown in Figure 13. A mixture of vapor, hydrocarbon condensate (mainly C1 to C5 chains), and water is first separated in a three-phase separator. Oily water from the separator is sent as a waste stream, the liquid hydrocarbon mixture is recovered as a product stream, and the vapor collected at the top of the separator is compressed and then condensed in a vapor condenser. To knock out more water and hydrocarbon from the condensed vapor, it is sent to a second three-phase separator. The vapor mixture from the second separator is then passed to a dryer to trap the water vapor, and the resulting dried hydrocarbon vapor is further compressed, condensed,

Table 5. Comparison between ENVOP Team's Results and That Generated by Applying the Systematic Waste Minimization Methodology

process unit	team's results	alternatives
dried HC vapor	less hydrocarbon feed to the plant	prevent excessive hydrocarbon feed, decrease temperature of hydrocarbon feed, use alternative feed rather than hydrocarbon in dried HC vapor stream
feed compressor	larger compressor power	increase the compressor power
vapor condenser	more cooling water flow rate, lower temperature of cooling water, use other coolant (glycol), larger heat-transfer area, add second cooler after heat exchanger	increase flow rate of cooling water, decrease temperature of cooling water, improve heat-exchanger design, use alternative cooling agent, use further cooling system after each cooler to convert more hydrocarbon vapor into liquid
flash separator	none	use further separation process after flash separator before going to flared HC stream to recover hydrocarbon vapor
flared vapor	recycling waste stream, use heavier hydrocarbon to absorb waste vapor, provide vapor recovery system after separator	direct recycling or recovery recycling of vapor waste stream

and separated as flared vapor and oil export. Actually, the downstream section of this process is the same as the compression–separation section shown in Figure 4 and discussed earlier. To aid the reader, the detailed steps that apply the systematic waste minimization methodology are elaborated using the compression–separation section and compared with the available experts' solutions. In the interest of space, only results derived from the methodology are presented for the entire hydrocarbon separation process case study.

The systematic waste minimization methodology proposed in this paper is applied to the compression–separation section. The environmental target for this section is to minimize the waste stream sent to the flare system. The first step is to identify the materials present in each unit and stream of the process. On the basis of the compression of the hydrocarbon vapor and the separation of the vapor and liquid hydrocarbon inside the flash separator, the material propagation in the process can be qualitatively simulated. The next step is to identify and diagnose the sources of each material component that make up the waste stream and to propose waste minimization alternatives accordingly. This is performed using the P graph model of the process. Figure 14 illustrates the P graph model for the compression separation case study with reference to each hydrocarbon vapor present in the waste stream. Waste minimization analysis based on this P graph model reveals that the presence of useful hydrocarbon vapor in the waste stream is mainly due to the excessive hydrocarbon fed to the process and the excess vapor that is not transformed inside the vapor condenser. The P graph model also reveals that the flash separator is not a critical unit because the vapor and the liquid hydrocarbon are separated effectively. On the basis of this diagnosis, the following top-level waste minimization alternatives can be derived: (1) prevent excessive hydrocarbon in the feed stream, (2) improve the design of the vapor condenser, (3) increase the condensation rate inside the cooler, and (4) use direct recycling or recovery recycling of the flared hydrocarbon stream.

The next step is to find detailed alternatives that focus on the vapor-condenser unit using the cause-and-effect knowledge. The digraph model of the vapor condenser reveals that increasing the pressure and lowering the temperature of the condenser would increase the condensation rate. Significantly, this means a reduction of the hydrocarbon vapor entering the flash separator and coming out as a waste stream. The functional model of this compression–separation section concludes that the cooling water stream and the dried feed vapor stream need to be modified accordingly because their functional variables, temperature and composition, directly affect the hydrocarbon vapor transformed inside the condenser. In the same way, the condensation inside the condenser is also dependent upon the temperature of the incoming feed stream. Using the functional model, this feed stream can be traced upstream until the dried feed vapor stream and, consequently, the alternative "decrease temperature of the dried feed vapor stream" can be derived. Similarly, the pressure of the compressor needs to be adjusted to increase the pressure in the flash separator for an increase in the bottom liquid recovery. Consequently, the cause-and-effect knowledge of the feed compressor gets activated in an appropriate manner, leading to alternative "increase compressor power".

A team of experts has carried out an ENVOP review of this compression–separation section. Table 5 presents the comparison between the team's findings with the ones obtained using our methodology.[23] As shown in the table, we are able to successfully identify and diagnose all of the sources of waste accurately and identify waste minimization alternatives by following the systematic methodology similar to the team's results. Waste minimization analysis of the entire hydrocarbon separation process (Figure 13) has also been carried out with respect to the following environmental targets: (1) reduce the flared vapor emission leaving the flash separator, (2) reduce oily water discharge from the three-phase separators, and (3) reduce the water vapor emission leaving the dryer unit.

Figures 15 and 16 show the P graph and functional models of the hydrocarbon separation process. As can be seen from the results tabulated in Table 6, the methodology is able to identify all of the sources of waste and appropriate waste minimization alternatives.

5. Conclusions

Waste minimization is gaining importance as the preferred means of pollution prevention. This two-part

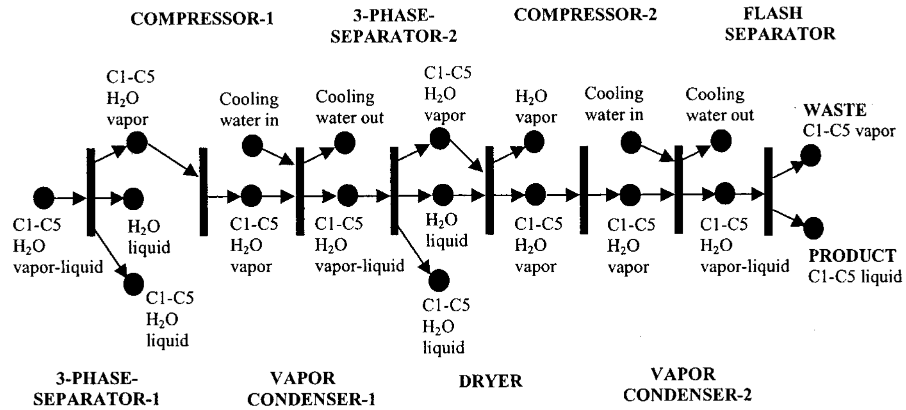


Figure 15. P graph representation of a hydrocarbon separation process.

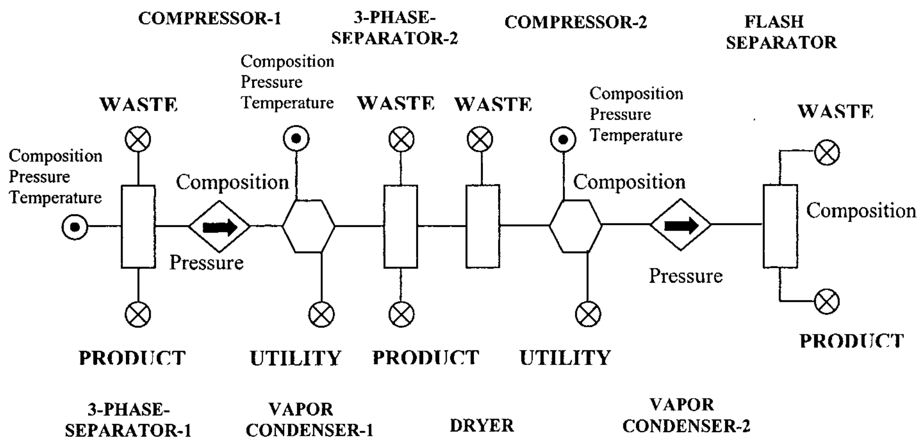


Figure 16. Functional model for a hydrocarbon separation process.

Table 6. Waste Minimization Alternatives for the Hydrocarbon Separation Process

process unit	alternative from waste minimization methodology
waste stream	direct recycle or recovery recycle of the useful material in the oily water streams and the flared vapor stream
separators	improve the design and control system of the dryer, three-phase separators, and flash separator, and use of further separation after each of the separators to recover more useful material before it is discharged as waste stream
compressors	increase the power of each compressor
condensers	use further cooling system after each cooler to convert more hydrocarbon vapor into liquid, increase the flow rate of cooling water to increase the condensation rate, decrease the temperature of cooling water to increase the condensation rate, improve the heat-exchanger design to increase the condensation rate, use an alternative cooling agent to increase the condensation rate
feed stream	prevent excessive hydrocarbon feed to decrease the useful material in waste stream, decrease the temperature of hydrocarbon feed, use an alternative feed rather than hydrocarbon in dried HC vapor stream, remove water impurity in the feed stream

paper presents a systematic methodology and a decision support system for a waste minimization analysis applicable to any chemical process plant. In part 1 of this two-part paper, the systematic methodology for qualitative waste minimization for waste diagnosis and analysis and alternatives generation has been proposed. This methodology utilizes three fundamental elements: a P graph, cause-and-effect model, and functional knowledge. An analysis based on the P graph provides a framework for obtaining top-level waste minimization alternatives, which can be further distilled to derive detailed options using digraph and functional knowledge. The methodology has been successfully tested on an industrial case study obtained from the literature involving a hydrocarbon separation process. The waste minimization solutions show that our proposed methodology is able to identify and diagnose the sources of waste accurately and generate waste minimization alternatives similar to those concluded by a human team performing an ENVOP review. Implementation of this methodology into an intelligent system with its application to a complex industrial case study will be discussed in part 2.

While the overall results from the methodology are very promising, the methodology by itself has some limitations. When multiple waste streams are present, multiple environmental impacts are generated from these streams and calls for trade-offs between the proposed alternatives and the impacts generated from each waste stream. For example, an alternative which targets a reduction in the emission from flared hydrocarbon may lead to increased organics loading in the aqueous waste stream. In general, this problem can be solved through quantitative assessment of the process (i.e., process variable changes and its overall environmental impact). We are currently exploring an integrated qualitative−quantitative approach that combines the waste identification and alternative generation capabilities of our methodology with the impact calculation assessment of the WAR (waste reduction) algorithm[24] for simultaneous evaluation of the economic and environmental impact of the process.[25,26]

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