Application of Artificial Intelligence Technique for Synthesizing of a Process for Waste Reduction

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***Abstract*— One of the most effective ways of minimizing wastes from their sources is to design an environmentally clean process which provides a satisfactory level of controllability. In the present work, a systematic module-based synthesis approach is developed to design such a process with minimal waste generation. This approach is featured by adding the dimension of structural controllability to the conventional capital and operating cost functions, and elaborating waste minimization strategies as constraints. Due to insufficient information and incomplete data regarding the mechanism of waste generation at the process design step, artificial intelligence techniques are utilized to represent waste minimization strategies and evaluate structural controllability. The efficacy of the proposed approach to waste minimization is illustrated by synthesizing a cost-effective and highly controllable process capable of minimizing phenol containing waste streams in an oil refinery**

Keywords—Waste synthesis,Minimization approach,In plant waste minimization stratagy,Module ased synthesis approach

I. INTRODUCTION

Rapidly changing industrial technologies are often accompanied by the increased generation of various hazardous or toxic wastes. The major portion of the wastes is mainly from chemical plant and petroleum refineries. These wastes, if improperly dealt with, can threaten both public health and environment. Consequently, waste rninimization and management (WMM) are a major concern of process engineers *(1-2)*. The EPA has established a waste priority hierarchy beginning in 1976 to promote better WMM alternatives. During last two decades, most of the effort on WMM has focused on waste incineration/treatment and land disposal. These are now the lowest priorities in EPA's hierarchy, due to the current emphasis on source reduction or in-plant pollution prevention. Recently, it has been recognized that the production of wastes from a chemical or petrochemical process is a function of process design and the manner in which the process is controlled and operated *(3-7)*. To effectively realize waste minimization (WM), it is beneficial to examine the basic characteristics of WM engineering in the process industry (Huang and Fan, *Intl. J. Computers in Industry,* in

(1) WM is a multi-disciplinary area involving engineering, chemistry, biology, fluid mechanics, mathematics, statistics, economics, and regulations;

thereby being a knowledge-intensive area. The acquisition and representation of the knowledge from the experts in these diverse fields is the focal point for successful WM.

(2) WM is heavily dependent on expertise. The behavior of a process generating wastes cannot be easily described by rigorous mathematical models. Qualitative analysis of the process is thus always necessary.

(3) The available information pertaining to WM is frequently uncertain, imprecise, incomplete, and qualitative in the design stage. Hence, standard

mathematical tools may be incapable of dealing with it.

(4) A large number of regulations and strategies for WM can be expressed as rules. The symbolic knowledge in the rules has to be appropriately represented and manipulated

Under these circumstances, it is very difficult, if not impossible, to resort to conventional algorithmic methods to design a process with minimal waste generation. On the other hand, artificial intelligence techniques such as knowledge-based approach and fuzzy logic are viable alternatives. The knowledge-based approach is powerful in acquiring both structured and

Un structured symbolic knowledge, and efficient in representing and manipulating them *(8)*. Today, numerical computation approaches can be embedded into a knowledge-based system to form a hybrid system. Fuzzy logic is capable of dealing with structured numerical knowledge and imprecise information, and provides a way to interpolate between regions with different rules *(9)*. A methodology incorporating the knowledge-based approach and fuzzy logic is thus highly advantageous

II. DESIGN PHILOSOPHY

With the recognition of the above basic characteristics of WM engineering, a design approach should have the following features:

(1) Early incorporation of the WM strategy. Process design consists of three major phases in sequence: synthesis, analysis/optimization, and detailed design; among them, process synthesis is the most abstract, therefore the most difficult phase. Clearly, the implementation of WM strategy in the later phases in process design, especially in the detailed design phase, is very limited, because waste generation caused by an improper process structure is extremely difficult to manage. It is desirable, therefore, to incorporate WM strategies starting from the earliest stage in process design, namely the pre analysis stage in process synthesis.

(2) Generic rather than problem specific. The design approach should be general enough to easily accommodate different restrictions on waste generation. These restrictions

may be on the generation of waste energy as well as waste species in different forms, such as gaseous, liquid, or solid. In an oil refinery, for instance, five major sources of generating hazardous or toxic wastes have been identified: process systems, power plant, storage and handling, waste water treatment, and miscellaneous *(10).* Among them, wastes from process systems are the most difficult to deal with due to complexity. When crude oil enters an oil refinery, it is a heterogeneous mixture of hydrocarbons and various impurities. Widely differing types of crude require different refining techniques and yield different product mixes. As by-products, a large amount of pollutants are generated from various processes. To minimize the generation of pollutants of these types, a general design approach is highly desirable.

In-Plant Waste Minimization Strategy

Even if a process is specifically designed for WM, the waste generated from it may still exceed a tolerable limit during its operation, due to not considering the effect of process structure on WM. Most processes experience disturbances with different intensities during operations. These disturbances can propagate in a process if disturbance propagation paths exist. Intense disturbance propagation inherited in the process structure may make tight control of the concentrations of hazardous species unattainable. Consequently, we need to synthesize a process which is not only cost-effective, but also highly controllable in terms of the quantity and toxicity of waste streams generated.

Representation of Waste Minimization Strategies.

The regulations and process designers' experience for WM are usually expressed in rule form. Various rules are available elsewhere *(2, 7,11,12).* These rules can be classified into the sets for: (i) measuring the toxicity of species, (ii) selecting a method for separating hazardous or toxic species, (iii) determining a separation sequence of stream components, (iv) evaluating the feasibility of recycling hazardous or toxic species, (v) selecting the strategies for recovering waste energy, (vi)implementing minimum capital and operating costs, (vii) enhancing structural controllability, (viii) modifying a synthesized process structure, and (ix) making a trade-off among capital cost, operating cost, and WM. While these rules are expressed in IF-THEN rule form, they need to be quantitatively represented. For instance, one rule is:

IF a process stream to a reactor contains hazardous Species,

THEN the species should be separated first before the stream enters the reactor in order to avoid the deactivation of catalyst in it.

This is a crisp rule in which no fuzziness is involved. Variables y_1 and y_2 are introduced to represent the species in a stream and the separation sequence of the hazardous species, respectively. Moreover, crisp sets $A1$ and A2 are defined as the set of hazardous species and that of hazardous species to be separated first, respectively. Two crisp membership functions can be defined below.

$$\mu_{A_i}(y_i) = \begin{cases} 1 & \text{if } y_i \in A_i \\ 0 & \text{if } y_i \notin A_i \end{cases} \qquad i=1,2 \tag{1}$$

Thus, the rule has the following two-valued logic expression.

$$A_1 \longrightarrow A_2. \tag{2}$$

However, many other rules are fuzzy in nature as illustrated below.

IF a process stream experiences severe disturbance of Mass flow rate at its inlet, AND the concentration of a species at the outlet of another stream must be controlled precisely to prevent pollutant generation,

THEN these two streams should not be matched in an extractor.

Since the imprecise information is involved in both premise and consequence of the rule, fuzzy set theory should be employed. Fuzzy variables Z_1, Z_2, and Z_3 can be defined as disturbance of mass flow rate of a stream, the fluctuation of the concentration of a species at the outlet of another stream, and the preference of matching these two streams, respectively. Correspondingly, three fuzzy sets, $B_{1,1}$, $B_{1,2}$and $B_{1,3}$, may be introduced to represent the concepts of severe, moderate, and slight disturbances, respectively.

$$\mu_{B_{1,1}}(z_1) = \begin{cases} 1 - 25z_1, & 0 \le z_1 \le M_1 \\ 0, & z_1 > M_1 \end{cases} \tag{3}$$

$$\mu_{B_{1,2}}(z_1) = \begin{cases} 25z_1, & 0 \le z_1 \le M_1 \\ 3 - 50z_1, & M_1 < z_1 \le M_u \\ 0, & z_1 > M_u \end{cases} \tag{4}$$

$$\mu_{B_{1,3}}(z_1) = \begin{cases} 0, & 0 \le z_1 \le M_1 \\ 50z_1 - 2, & M_1 < z_1 \le M_u \\ 1, & z_1 > M_u \end{cases} \tag{5}$$

imilarly, fuzzy sets $B_{2,1}$, $B_{2,2}$ and $B_{2,3}$ should be defined to represent the concepts of high, moderate, and low control precision of species concentration, respectively. Fuzzy sets B3 χ and B3 2 must be designated according to the concepts of preferred and not preferred stream match, respectively. The fuzzy rule can thus be expressed by the following fuzzy logic form.

$$\wedge \{B_{i,j} \mid i=1,2;\ j=1,2,3\} \longrightarrow \wedge \{B_{3,k} \mid k=1,2\} \tag{6}$$

Classification of Process Information. The representation of WM strategies, as described in the preceding section, indicates that process information directly influencing WM must be carefully classified. This includes the disturbances of temperature, pressure, mass flow rate, and species concentration at the inlets of process streams , as well as the tolerable ranges of the fluctuation of concentrations of hazardous species at the outlets of process streams. In a separation process, for instance, for each stream i, a disturbance of source concentration of waste species Ps,$^{\delta}Y_{pi}^{s}$ in both positive and negative directions, and that of mass flow rate, $^{\delta}M_i$ also in both directions, lead to a change in mass flow rate of the species ρ, δ, M_{pi}.

$$\delta M_{p_i} = \max\{|M_i \delta y_{p_i}^{s(+)} - \delta M_i^{(+)}(y_{p_i}^{t} - y_{p_i}^{s})|, \\ |M_i \delta y_{p_i}^{s(-)} - \delta M_i^{(-)}(y_{p_i}^{t} - y_{p_i}^{s})|\} \quad (7)$$

This example shows that different types of disturbance variables may be lumped into a single variable, which simplifies the quantification of the overall influence of all related disturbances. Generally, the more intense the disturbances in the input variables, the greater the deviation in the output variables from their normal values. Based on their magnitudes, the disturbances can be classified into a number of degrees, such as *very slight, slight, moderate, severe,* and *very severe* disturbances. The degrees are quantified by fuzzy sets as illustrated in Figure 1. Usually, it is unnecessary to control all output variables of a process to the same level of precision. For example, the composition of a highly toxic species of a stream must be controlled very tightly, while that of a non-toxic component of a stream is less critical. Based on the complexity of a WM problem, the control precision of the output variables can be divided into several grades, such as ***very low, low, moderate, high,*** **and** ***very high.***

The quantification of levels of control precision is similar to that described above. A disturbance at the inlet of a stream must propagate to the outlet of another stream if a downstream path exists *(13).* When the two streams match directly through a process unit, the effect of this disturbance on the outlet of another stream is quick and drastic. When they match indirectly through two process units, such an effect is slower and moderate. When the disturbance propagates through many process units before reaching an outlet, its effect dissipates. The more the number of process units involved in disturbance propagation, the greater the extent of dissipation of disturbance influences. The patterns of disturbance propagation can be defined based on the type of a process system. In an exchanger network, four patterns *(very severe, severe moderate,* and *negligible* propagation) can be introduced, depending on the number of process units through which a disturbance travels *(14).*

The patterns of disturbance propagation in a process can be illustrated by the example in Figure 2. This mass exchanger network (MEN) contains four mass-exchange-based process units (e.g., an extractor, an absorber, or an absorber for recovering hazardous species) as illustrated by the grid diagram of Figure 2a. In this figure, the degree of a disturbance caused by the fluctuations of concentration and/or mass flow rate is indicated by the number of solid circles, "•"'s. For instance, symbol "••" represents moderate disturbance.

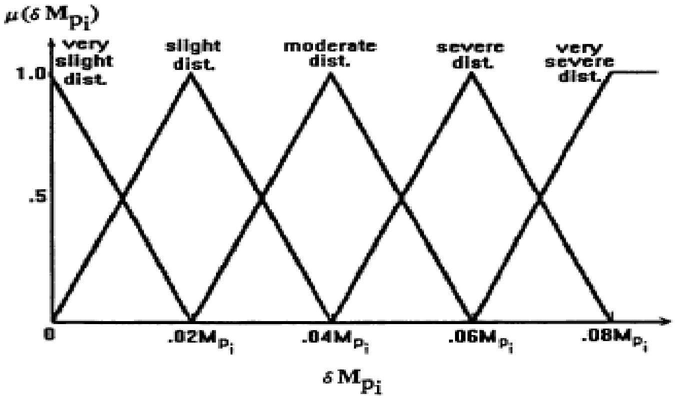
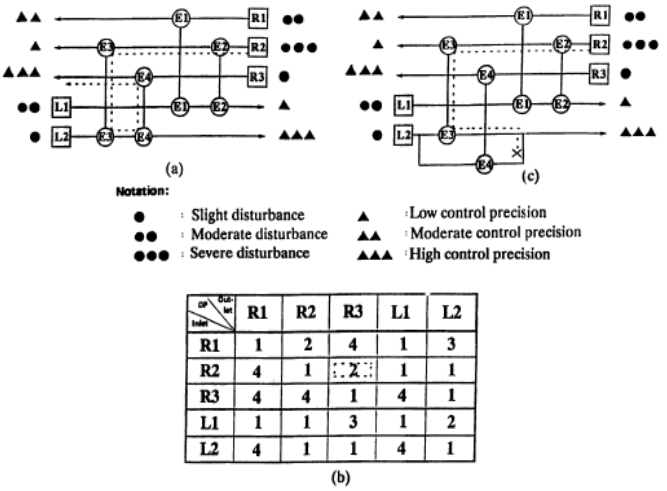


Figure-1: Quantitative representation of fuzzy linguistic terms, VERY SLIGHT, SLIGHT, MODERATE, SEVERE, and VERY SEVERE DISTURBANCES



Out-let Inlet	R1	R2	R3	L1	L2
R1	1	2	4	1	3
R2	4	1	2	1	1
R3	4	4	1	4	1
L1	1	1	3	1	2
L2	4	1	1	4	1

Figure-2: Disturbance propagation through a mass exchanger network and modification of the network structure

The precision level of control at a stream outlet is indicated by the number of triangles, "▲"s. For example, the symbol "▲▲▲" represents high control precision. All patterns of disturbance propagation involved are listed in the disturbance propagation table of Figure 2b. The first column of the table designates the inlets of the five streams; the first row designates their outlets. Each integer in the renaming entries of the table represents the pattern of disturbance propagation. For example, a disturbance exerted at the inlet of rich stream R2 propagates through process units 3 and 4, and reaches the outlet of rich stream R s . In this disturbance propagation path, two process units are involved. According to the definition, this is severe propagation (pattern-2), and thus an integer of 2 is assigned to entry (R2, R3). This disturbance propagation is undesirable since the species concentration at the outlet of rich stream Ra should be controlled very precisely, but it is constantly disturbed by a severe disturbance from rich stream R s . This WM problem due to improper process structure can be resolved in a number of ways. The process modification in Figure 2c is one possible solution if it is thermodynamically feasible. In this solution, the stream splitting terminates the disturbance path from rich streams R2 to Ra with a negligible increase of capital cost and no increase of operating cost.

III. STUCTURAL CONTROLLABILITY

The degree of structural controllability of a process reaches a maximum when the occurrences of undesirable disturbance propagation and their severities are at a minimum, thereby minimizing the possibility of waste generation due to the process structure. Thus, the structural controllability can be assessed by examining the patterns of disturbance propagation through the process. To evaluate it quantitatively, it is convenient to define a disturbance vector D, control precision vector C, and disturbance propagation matrix P for a process having N streams. D comprises all existing disturbances which are detrimental to WM. Each element, d{, in D represents the intensity of a disturbance exerted at the inlet of stream i. C specifies the levels of control precision required for all output variables. Each element, Cj, in C represents the control precision required at the outlet of stream j. P lists all disturbance propagation in the process. The value of element P_{ij} in P corresponds to the intensity of the propagation. Each element in D, C, kid FIS quantitatively evaluated by fuzzy set theory as discussed previously. To facilitate the evaluation of structural controllability in terms of WM, and to compare various process flow sheets, the index, Isc, is created which has the following general form.

$$I_{sc} = \frac{E_{tot,max}(D,C,P) - E_{tot}(D,C,P)}{E_{tot,max}(D,C,P) - E_{tot,min}(D,C,P)} \qquad (8)$$

Where $E_{tot,max}$(D,C,P) and $E_{tot,min}$(D,C,P) chararacterize a process with maximum disturbance propagation,rescectively. Consequently, the former is the least controllable with the minimum generation of waste which is definitely undesirable: the later is the most controllable with the minimum generation of waste which is also undesirable due to extremely high capital and operating costs. In fact, to completely eliminate waste generation in a process plant is usually unreachable.

Our goal is to design a highly controllable process which is characterized by the terms, Etot(D,C,P). For a separation process using extractors, absorber, and distillation columns or an energy recovery process using heat exchangers, the index can be found in *(14).*

Module-Based Synthesis

For the knowledge extracted and formalized thus far to be practical, it is imperative that a stage wise procedure for the synthesis be developed; in other words, the knowledge represented in the preceding sections should be systematically organized. Following the three stages in process synthesis, the synthesis procedure consists of three major modules, associated with a number of additional modules to perform specific tasks. The relationships of these five modules are illustrated in Figure 3.

Pre analysis Module

The major function of the pre analysis module includes the estimation of both of capital and operating costs and making decisions on stream matching which should lead to the least waste generation. The costs are estimated by pinch technology *(11).* In the present work, capital cost is approximated by counting the total number of process units, a heuristic which is commonly used in process synthesis. For a synthesis problem, process input and output variables are to be identified; process data including normal operation point and fluctuations are analyzed and classified by the approach in the preceding sections. After classification, a waste minimization assessment table is constructed by activating the waste minimization enhancement module. The values of certain grids, i.e., the values of the element p.. in the disturbance propagation matrix P, must be pre-assigned in the table according to the rules generated for implementing WM strategies. Such a WMA table is termed the admissible WM table. The pre-assignment of values to these grids implies the most favorable and the least favorable decisions on placement of process units.

Structure Invention Module. A series of decisions is made on the selection and placement of process units to match pairs of process streams. Each decision's effect on the WM is assessed through evaluation of the index of structural controllability, Is c. Note that each stream match directly introduces disturbance propagation path, which may influence WM. The recommendations of the locations of process units to be placed, which are reflected in the admissible WM table, should be adopted gradually. Several sets of rules for reducing the total cost and improving WM are applied to ensure the identification of an optimal solution. This module needs to repeatedly activate the waste minimization enhancement module and the stream matching mod

Structure Evolution Module

The resultant process flow sheet is examined by the structure evolution module. Usually, when a number of separately synthesized sub-systems in the structure invention module are combined to form a complete process, two undesirable situations may occur:

(1) the total number of process units exceed the minimum requirement, and

(2) the WM may deteriorate due to newly introduced intense disturbance propagations.

Hence, trade-offs need to be made among the number of process units, energy or material consumption, and WM characterized by structural controllability. The trade-off is usually based on engineering judgment. The preference in this work is given to the prevention of intense disturbance propagation to the process streams whose outlet concentrations of hazardous species need be controlled very precisely.

Waste Minimization Enhancement Module

In this module, the admissible WM table needs to be constructed to impose restrictions on stream matching to prevent undesirable disturbance propagation. The main part of the table is disturbance propagation matrix P as discussed in the preceding section. In the table, some elements of P have pre assigned values corresponding to either preferred or disallowed stream matches. Note that at the pre analysis stage, it is impossible to assign values to all elements in the table because of the lack of knowledge about the detailed interconnections among streams through process units. In the procedure, a value of “l" of the element, Pj j, represents the unavoidable very severe propagation (pattern-1) originating from the inlet of stream i to its own outlet. A value of T of the element, P_{ij}, $i \neq j$, implies a direct match between streams i and j, which yields two pattern-1 disturbance propagation. This assignment is made according to the intense-propagation diverting rule and minor-propagation-introducing rule. Note that the match introduced should be thermodynamically feasible. This type of match is useful for diverting severe disturbance propagation to a stream whose hazardous species concentration needs to be controlled precisely. Thus, waste generation can be effectively restricted.

A value of "0" to the elements, P_{ij}, $i \neq j$, implies that an indirect match will lead to a downstream path spanning at least four process units; this is negligible propagation (pattern-4). This assignment represents the complete or almost complete isolation between streams i and j. Thus, a disturbance of stream i cannot propagate to the outlet of stream j. This is, in fact, a type of strict constraint on waste generation.

The values of "0.5" and "0.25" represents the restrictions on the path length of disturbance propagation between a pair of streams. The value of "0.5" indicates that the two streams are connected through at least two process units; it corresponds to pattern-2 propagation. The value of "0.25" implies that the two streams are linked through at least three process units; it corresponds to moderate propagation (pattern-3). The assignment of these different values to certain elements in matrix P also enhances WM through controlling disturbance propagation.

Stream Matching Module

The selection of a stream match from a set of match candidates is always based on the information provided by the WMA and the admissible WM tables. Each match candidate needs to be evaluated according to fuzzified heuristic rules. A candidate with the highest priority is always selected. Although it is problem specific, a general procedure for applying the heuristic rules is developed.

IV. APPLICATION

The approach has been successfully applied to synthesize a mass exchanger network (MEN) for minimizing phenol waste in an oil refinery. Phenolics are considered to be one of the major organic toxic species that should be minimized in waste streams in a refinery. Phenol-containing waste streams are generated from a number of processes in an oil refinery, such as a phenol solvent-extraction process and a catalytic cracking process *(15).*

Problem Analysis

In the phenol solvent-extraction process, the waste stream leaving the process usually contains excessive phenol. These streams essentially come from three process units, i.e., raffinate tower, water/phenol tower, and extract stripper as illustrated in Figure 4. Conventionally, these streams are mixed first and then enter an absorber in which heated lubricating oil stocks absorb phenol from them *(15).* In reality, the temperature, compositions, and flow rates of these streams are always different, and the fluctuations of these variables are stream independent. Consequently, mixing these streams is thermodynamically inefficient.

A mass balance computation indicates that lubricating oil alone is incapable of reducing the phenol concentration in the mixed stream to a tolerable range 0.002). This is especially true when severe disturbances appear at the inlet of the stream. Consequently, a MEN is desirable to reduce the concentration of phenol species regardless of the existence of various disturbances.

While a family of solvents can be used for recovering phenol, activated carbon is utilized in this case; however, the minimum quantity of activated carbon is expected to reduce the total cost. The process data for the synthesis problem is in Table I. Three streams from the raffinate tower, water/phenol tower, and extract stripper are designated rich streams R i , R2, and R a , respectively; the lubricating oil and activated carbon are lean streams L i and L 2 , respectively. Note that the mass flow rate and phenol concentration at the outlet of stream L2 in the table are the upper limits. The intensity of disturbances appearing at the inlets of streams and the requirement of control precision of phenol concentrations at the outlets of streams are also specified. The target is to synthesize a cost-effective and highly controllable MEN. The pinch point is located at the lean end of the composite curve in a concentration-mass load of phenol species diagram. The minimum number of process units to be utilized is five. The minimum consumption of mass separating agent (MSA) is 0.0681 kg

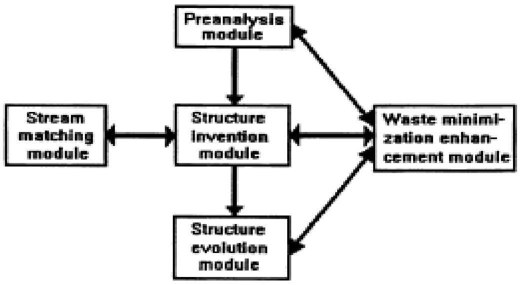


Figure-3: Connection mode of the modules in a synthesis procedure

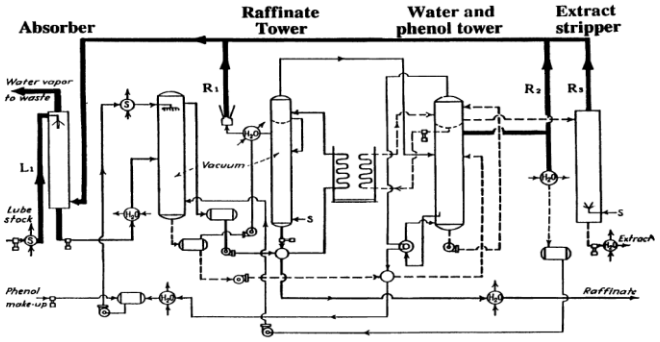


Figure-4: Phenol solvent-extraction process

V. SOLUTION AND COMPARISON

By the present approach, an optimal solution of the synthesis problem, i.e., solution A, is identified in Figure 5. This MEN contains three absorbers and two adsorbers which are the minimum number of process units. The consumption of activated carbon also reaches the minimum.

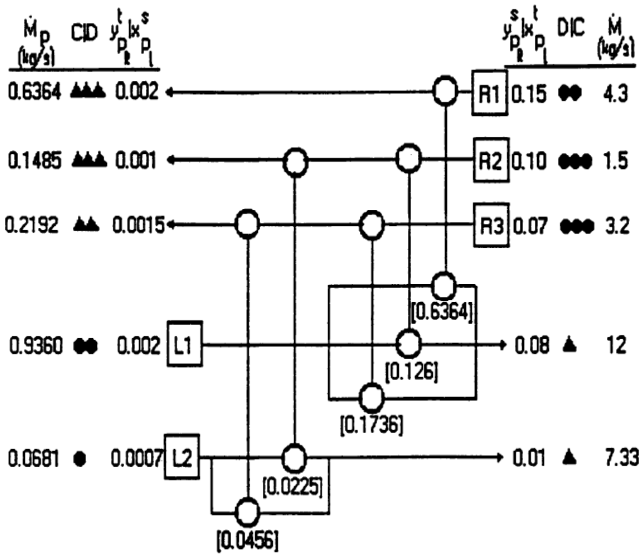
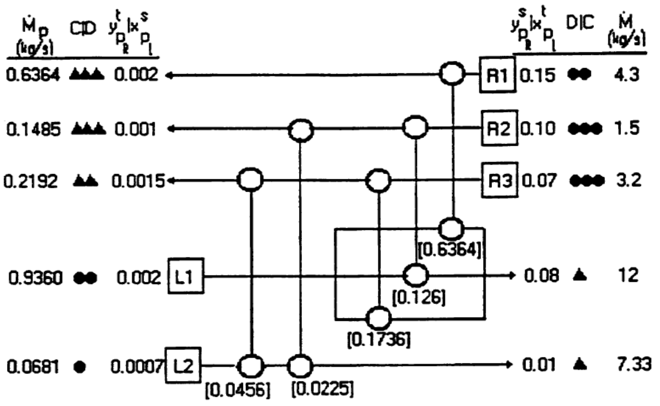
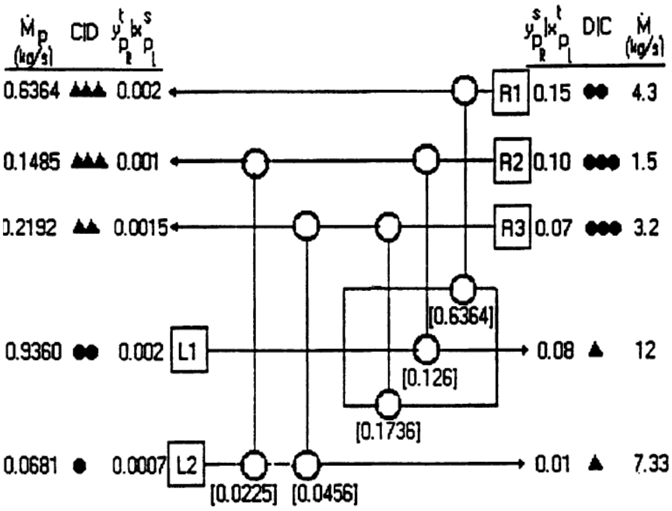


Figure-5:Optimal mass exchanger network for minimizing phenol species waste streams (identified by the AI approach

Moreover, it is highly controllable. To demonstrate the superiority of the solution, two types of exhaustive search are conducted. For the first type of search, the same restrictions are imposed as those used in identifying a solution in Figure 5. Three solutions of this type are identified. One is the same as the solution structure in Figure 5, and the other two, named E-l-a and E-l-b, are depicted in Figures 6a and b, respectively.



E-1-a



E-1-b

Figure-6:Mass exchanger networks for minimizing phenol species in waste streams (Identified by the first type of exhaustive search)

The second type of search is performed by imposing only one restriction, i.e., the minimum number of process units. In this case, the consumption of MSA is allowed to exceed the minimum requirement, if a process is highly controllable. With these restrictions, a large number of solutions are identified. The superiority of solution A in Figure 5 over the other two solutions E-l-a, E-l-b can be understood through examining their structures. In this synthesis problem, two intense disturbances exist at the inlets of rich stream R2 and R s. The concentration of phenol species at the outlets of rich stream R i and R2 should be controlled very precisely, and that of Rs should be controlled moderately. In solution A, these two intense disturbances at R 2 and R s cannot propagate to the outlets of Ri and R2 , respectively ; the intense disturbance at R2 is not able to reach the outlet of R s . Thus, the target concentrations 0.002) of phenol species in Ri,R2,and Rs can be effectively controlled. By contrast, the intense disturbance at the inlet of R s will propagate to the outlet of R2 in structure E-l-a; the intense disturbance at the inlet of R2 will reach the outlet of R s in structure E-l-b. Clearly, these four solutions are structurally undesirable.

The five solutions are compared in terms of the consumption of MSA, the number of process units, and WM capability which is reflected by the degree of structural controllability. As summarized in Table Π, solution A is clearly the best one. The phenol concentrations of streams leaving the MEN can be strictly controlled to the minimum while yielding the minimum cost. Concluding Remarks Waste minimization and management are becoming the key issues today in chemical and petrochemical industries in complying with the regulations of environmental protection. To effectively minimize waste from sources in these industries, one of the most important ways is to evaluate the existing process structures and modify them if necessary, or design certain sub-processes. An artificial intelligence approach has been developed in this work for this purpose. By this approach, broad knowledge required for the design activity, whether it is

symbolic or numeric, can effectively be acquired, represented and manipulated, thereby facilitating the design of a cost-effective process with minimal waste
generation. The efficacy of the approach has been demonstrated by designing a mass exchanger network for minimizing phenol waste streams in an oil refinery.
This approach is currently being applied to the modification of a process to minimize hydrogen sulfide species in waste streams, also in an oil refinery.

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