

Simulated Annealing Approach to the Optimal Synthesis of Distillation Column with Intermediate Heat Exchangers

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Abstract This article presents a simulated annealing-based approach to the optimal synthesis of distillation column considering intermediate heat exchangers arrangements. The number of intermediate condensers and/or intermediate reboilers, the placement locations, the operating pressure of column, and the heat duties of intermediate heat exchangers are treated as optimization variables. A novel coding procedure making use of an integer number series is proposed to represent and manipulate the structure of system and a stage-to-stage method is used for column design and cost calculation. With the representation procedure, the synthesis problem is formulated as a mixed integer nonlinear programming (MINLP) problem, which can then be solved with an improved simulated annealing algorithm. Two examples are illustrated to show the effectiveness of the suggested approach.

Keywords distillation, intermediate heat exchanger, synthesis, mixed integer nonlinear programming, simulated annealing

1 INTRODUCTION

Distillation is one of the most common separation operations in the process industries, but is also known to be an energy-consuming and sometimes thermodynamically ineffective operation. One of the effective methods for saving energy in a distillation column is the use of intermediate condenser and/or intermediate reboiler. Zodonik presented an example of an ethylene plant where the use of an intermediate reboiler near the middle of a deethanizer column led to energy savings with a payback period for the added equipment of much less than one year [1]. Patterson and Wells presented another distillation example to show the benefits of the intermediate reboiler [2]. In sub-ambient distillations, the use of intermediate reboilers and condensers to reduce energy consumption is well known [3]. Agrawal *et al.* presented analysis methods that lead to quick identification of the binary distillations for which an intermediate reboiler or condenser can lead to a substantial improvement in thermodynamic efficiency [4–8]. The simulation and experimental study of intermediate heat exchanger in a sieve tray distillation column has been presented by Ingela *et al.* [9]. However, it is noted that, as far as is known, nearly all the previous publications related to the type of distillation scheme were based on thermodynamic analysis and simulation comparisons. With these methodologies, the structure decision was often based on rules of thumb or on an exhaustive enumeration of all the possibilities. To overcome these disadvantages, the article presents an algorithmic approach for solving the addressed synthesis problem.

Generally, the problem of synthesizing distillation column with intermediate heat exchangers includes two aspects. One is to find an optimal distillation configuration and the other is to determine the optimal operating parameters of the column so as to arrive at the minimum overall cost for the system.

Mathematically, the synthesis problem can be formulated as a mixed integer nonlinear programming (MINLP) problem. However, the high-nonlinearity of the model makes deterministic optimization methods inefficient and unlikely to be successful. On the other hand, stochastic optimization strategies have been known to solve a large class of nonlinear problems to global optimization.

Simulated annealing (SA) algorithm is a well-established stochastic search technique for the combinatorial optimization [10, 11]. In the previous studies, an improved SA algorithm for the synthesis of heat integration complex distillation system has been systematically developed [12–15]. The developed approach has two robust characteristics. First, the structural decisions of the problem can be described directly by a coding procedure that allows the use of more rigorous evaluation methods for process design; Second, SA algorithm was improved so that it could handle structural and parametric optimization simultaneously within the same annealing scheme. As a consequence, the complexities of formulation and handling of an explicit MINLP model can be avoided. In this study, the approach is extended to the problem of synthesizing distillation column with intermediate heat exchangers.

2 PROBLEM STATEMENT

The problem addressed in this article can be stated as follows.

Given a single feed mixture of known condition, which is to be separated into overhead and bottom products of specified compositions, the problem is then to synthesize an optimal distillation column configuration allowing the use of intermediate condensers and/or intermediate reboilers arrangement to satisfy the criteria of minimum total annual cost.

In this synthesis framework, the structural decisions consist of: ① the number of intermediate reboilers

and /or intermediate condensers; ② the placement locations of intermediate heat exchangers; ③ the match structure between utility levels and heat exchangers. The continuous variables are the operation pressure of column and the heat duties of intermediate heat exchangers. The main assumptions made for column design will be discussed later in this article (Section 4).

3 STRUCTURE REPRESENTATION

This section presents a comprehensive structure representation to which the stochastic search techniques are applied. The approach is based on a coding procedure that makes use of an integer number series to represent and manipulate the structural decisions of system. Here, the main steps of the approach are given below.

Consider a distillation column with N stages not including a base (top) condenser and a base (bottom) reboiler. The order of stages is specified from the top to the bottom. Two integers N_r and N_s are used to denote the number of stages in rectifying section and stripping section, respectively. Suppose that each stage is allowed to place an intermediate heat exchanger, excluding the feed stage, the base condenser and the base reboiler.

The utility conditions considered in this study includes: ① a set of cooling mediums with N_C different temperature levels represented with $U_C = \{1, 2, \dots, N_C\}$; ② a set of heating mediums with N_H temperature levels represented with $U_H = \{1, 2, \dots, N_H\}$. For all of the heat exchangers in a column, the feasible utility levels need to be selected to match them.

3.1 Generation of intermediate heat exchanger structures

3.1.1 Encoding procedure

A code-based procedure is introduced in this step to draw all possible intermediate heat exchangers structures (*i.e.* superstructure). The procedure is based on defining two integers (X and Y), $X \in [0, 2^{N_r} - 1]$ and $Y \in [0, 2^{N_s} - 1]$, which are capable of representing all the states of intermediate condensers in rectifying section and intermediate reboilers in stripping section, respectively. The advantages of the representation are

that: ① the two integers can be treated directly as the discrete (structural) variables of problem; ② the transformation of a structure to another neighboring one by using SA algorithm purely becomes the modification of integers X and Y within their feasible ranges.

3.1.2 Decoding procedure

The step is performed by converting integers X and Y to their equivalently binary digits, which is further used to identify whether the existence or non-existence of an intermediate condenser or reboiler for each stage. By performing the transformation, for integer X , a corresponding binary sequence $\{\varphi_i\} (i = 1, 2, \dots, N_r, \varphi_i \in \{0, 1\})$ is obtained, and for integer Y , $\{\beta_j\} (j = 1, 2, \dots, N_s, \beta_j \in \{0, 1\})$ is obtained. Note that the length of code elements in $\{\varphi_i\}$ and $\{\beta_j\}$ arranged is the same as the number of stages in rectifying section (N_r) and in stripping section (N_s) so that a one-to-one correspondence between a stage and a code (0 or 1) can be created. The further specifications made are: if $\varphi_i = 1$, it denotes an intermediate condenser in stage i , and conversely, if $\varphi_i = 0$, it denotes no intermediate condenser in stage i ; similarly binary sequence $\{\beta_j\}$ can be used for representing intermediate reboiler in each stage of stripping section. With the decoding procedure, a specific intermediate heat exchanger structure can be identified by performing a search program from first stage to the last one.

The above-presented steps are illustrated with an example as shown in Fig. 1. In this example, a base column with $N_r = 6$ and $N_s = 7$ is assumed as shown in Fig. 1 (a). Two integers $X = 49$ and $Y = 27$ are illustrated to represent an initial state of column structure, which can be represented equivalently as two binary sequences $\{\varphi_i\} = [110001]$ and $\{\beta_j\} = [0011011]$ as shown in Fig. 1 (b). By performing the proposed identification algorithm, the one-to-one correspondence between a stage and the existence or nonexistence of intermediate heat exchanger can be easily identified as shown in Fig. 1 (b) (where IC and IR refer to an intermediate condenser and an intermediate reboiler, respectively).

3.2 Constraints of structure's feasibility

It should be pointed out that, although it is possible

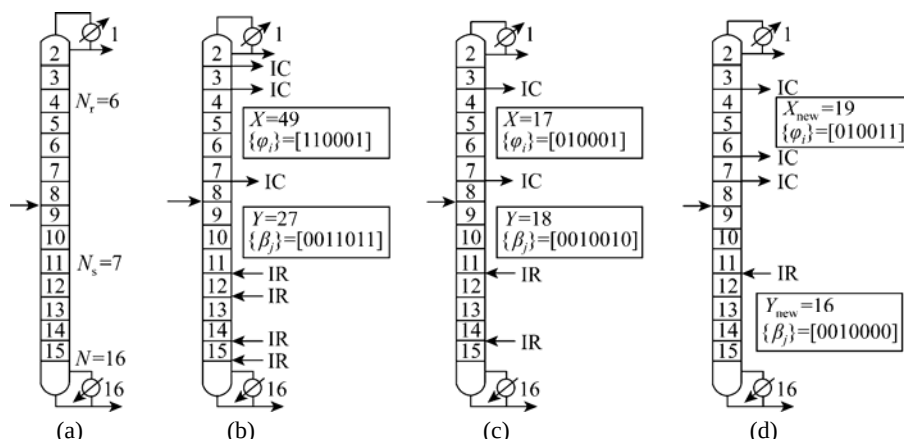


Figure 1 An illustrated coding procedure. (a) a base column; (b) an initial structure; (c) a structure of eliminating unfeasible intermediate heat exchangers; (d) a neighboring structure

to install intermediate heat exchangers at numerous locations in the distillation column, it is theoretically possible but seldom practical to apply this concept to each stage from the viewpoint of economics and operability. Based on this, the following three rules based on the heuristic of Douglas [16] are applied for problem constraints.

Rule a. The placement of an intermediate heat exchanger must meet the requirement of the minimum heat transfer temperature difference. A fixed value of 10 K is set in this article.

Rule b. For an intermediate condenser (reboiler) installed, if its operating temperature allows only the use of a cooling (heating) medium, the same as that used in the base condenser (reboiler), the intermediate condenser (reboiler) is discarded.

Rule c. If there are more than one intermediate heat exchanger set between two adjacent temperature levels of utility, only one of them is reserved based on the heuristic of Douglas [16].

By applying the above-mentioned rules, a set of intermediate heat exchangers will be discarded from the initial state of structure. Accordingly, their corresponding code element 1 in binary sequences will be replaced by 0. The approach is illustrated as shown in Fig. 1. It is supposed that an intermediate condenser placed in stage 2 and two intermediate reboilers placed in stages 12 and 15 are forbidden. The corresponding state of structure is then replaced as shown in Fig. 1 (c).

3.3 Generation of neighboring structures

In applying a SA algorithm, each new neighboring structure needs to be generated in a random way. Due to the proposed approach using two integers X and Y to represent structural variables of the problem, the generation of a neighboring solution can be simply achieved as follows:

$$X_{\text{new}} = \begin{cases} X + H & \text{if } r > 0.5 \\ X - H & \text{if } r < 0.5 \end{cases} \quad (1)$$

$$Y_{\text{new}} = \begin{cases} Y + L & \text{if } r > 0.5 \\ Y - L & \text{if } r < 0.5 \end{cases} \quad (2)$$

where X_{new} and Y_{new} refer to neighboring solution of X and Y , respectively. r is a pseudo-random number distributed between 0 and 1. H and L are the other two integers representing a search step-length whose values can be adjusted for a specific problem. The approach is also illustrated as shown in Fig. 1, by setting a step-length of 2, a neighboring structure, Fig. 1 (d) is generated from its original structure of Fig. 1 (c).

3.4 Generation of utility matches for intermediate heat exchangers

In this proposed structure representation, the match structures between intermediate heat exchangers and utility levels available are also treated as the structural decisions. Due to the discrete characteristic of utility levels, a code-based approach is also used to

represent them.

In rectifying section, the match structure can be represented as $M_C = \{i, m\} (i = 1, 2, \dots, N_r, \varphi_i = 1, m \in \{U_C\})$ (cooling medium m matches a intermediate condenser in stage i). Similarly, in stripping section the match structure can be represented as $M_H = \{j, n\} (j = 1, 2, \dots, N_s, \beta_j = 1, n \in \{U_H\})$ (heating medium n matches a intermediate reboiler in stage $N_r + j$).

4 COLUMN DESIGN AND COST CALCULATION

When a structural code has been generated, that is the configuration of a distillation column is given, the second step is to optimize the parameters to obtain a minimum total annual cost. In this study, the operating pressure of column and the heat duties of intermediate heat exchangers are treated as continuous decisions, and a stage-to-stage calculation method proposed by Lewis and Matheson is applied for column design [17].

The way of placing intermediate heat exchangers to a distillation column adopted in this study is the same as that in Agrawal and Herron [4]. For an intermediate reboiler (condenser) placed in a column, it is assumed that all the liquid (vapor) is withdrawn from a stage in stripping (rectifying) section and is then partially vaporized (condensed) through an intermediate reboiler (condenser) and return to its adjacent stage. It is assumed that the intermediate heat exchanger operates adiabatically and the phases leaving the intermediate heat exchangers are in equilibrium. With these assumptions, designing a column with intermediate heat exchangers can be carried out by combining a stage-to-stage method with a set of flash calculations.

The main assumptions made in this article are in accordance with that in Agrawal and Herron [4]. To simplify the calculating procedure, the reflux ratio in distillation column is held constant. The k -values, enthalpies and associated thermodynamic properties in each separation stage are calculated with Peng & Robinson EOS. The parameters obtained in this level include the number of stages, feed locations, temperature, compositions profiles and so on. The optimum obtained in this level can then be subjected to a more detailed design and rigorous simulation. The economic evaluation adopted in this study is based on the total annual cost, and all parameters related to cost calculation are taken from Guthrie [18].

5 MINLP MODEL AND SOLUTION

Based on the above-mentioned study, the problem can be described by the following MINLP concept model:

$$\min \text{COST} = \min C(X, Y, M_C, M_H, p, q_{IC}, q_{IR})$$

where p is the operating pressure of column, q_{IC} and q_{IR} refer to heat duty of intermediate condensers and reboilers, respectively. All these continuous variables are constrained by their bound conditions. Due to the

optimization model including discrete and continuous variables simultaneously, it forms a MINLP problem.

The presented model is solved by an improved SA algorithm suitable for MINLP optimization that was previously developed. This article does not represent specifically the implementation of the algorithm; for more details about, refer to An [19].

6 ILLUSTRATION EXAMPLES

6.1 Example 1

A binary separation problem taken from Luyben [20] is used here to show the principles of the developed synthesis procedure. The feed conditions and separation requirements are given in Fig. 2. The utility levels available are listed in Table 1.

Table 1 The available utilities

Utilities	Temperature/K	Price based on 1 t/dollars
1. cooling water	305.15	0.1323
2. ammonia 1	274.15	6.4511
3. ammonia 2	255.15	10.4324
4. ammonia 3	251.48	11.4567
5. steam 1	376.15	5.0274
6. steam 2	410.15	6.1740
7. steam 3	453.15	7.4970
8. steam 4	480.15	8.2026
9. steam 5	523.15	9.9666

First, the design and optimization of a base distillation column without intermediate heat exchanger is carried out. The optimum obtained in this step is given in Fig. 2 (a). Second, the synthesis problem considering intermediate heat exchangers is solved

and an optimal solution is located as shown in Fig. 2 (b). With the representation, the optimal solution is featured as $Y = 163$, $\{\beta_j\} = [10100011]$, $M_H = [(38, 3), (41, 4), (55, 5)]$ (note that the former code indicates stage while latter indicates code name of heating stream levels). This problem is solved with the proposed approach within 40 iterations and with about 70 s of total CPU time using an IBM compatible PC (Pentium IV/2.8G). The evolution of the calculation is shown in Fig. 3. It can be seen that a number of local optima are jumped off during the simultaneous evolution of the two types of variables, and in the later part of the evolution course, the curve becomes smooth due to the fact that the algorithm gives more chances for the evolution on the continuous parameters. Also, it was found that starting from different initial solutions, the same optimum, Fig. 2(b), is always located, which shows the good adaptability of the presented approach.

In Fig. 2 (b), two intermediate reboilers, IR 1 and IR 2, are allowed to be placed in stages 38 and 41, respectively, which leads to a saving of the total annual cost of 9.42% as against of the conventional base column. The saving, according to the calculation, is contributed to two aspects. In the first, the consumption of high-pressure heat stream used in base reboiler is reduced significantly due to the use of two cheaper levels of utility steams for intermediate reboilers, which leads to a saving of the operating cost about 11.31%. In the second, the column diameter is reduced owing to the decrease of vapor rates in column using intermediate reboilers, which offsets the increase of added equipment and leads to a saving of capital cost about 0.57%. From the results obtained, the necessity of considering intermediate reboilers for the illustrated example is demonstrated.

Luyben [20] studied the same separation example aiming at the problem of design and dynamic controllability of distillation column with intermediate reboilers. The basic method adopted in this published

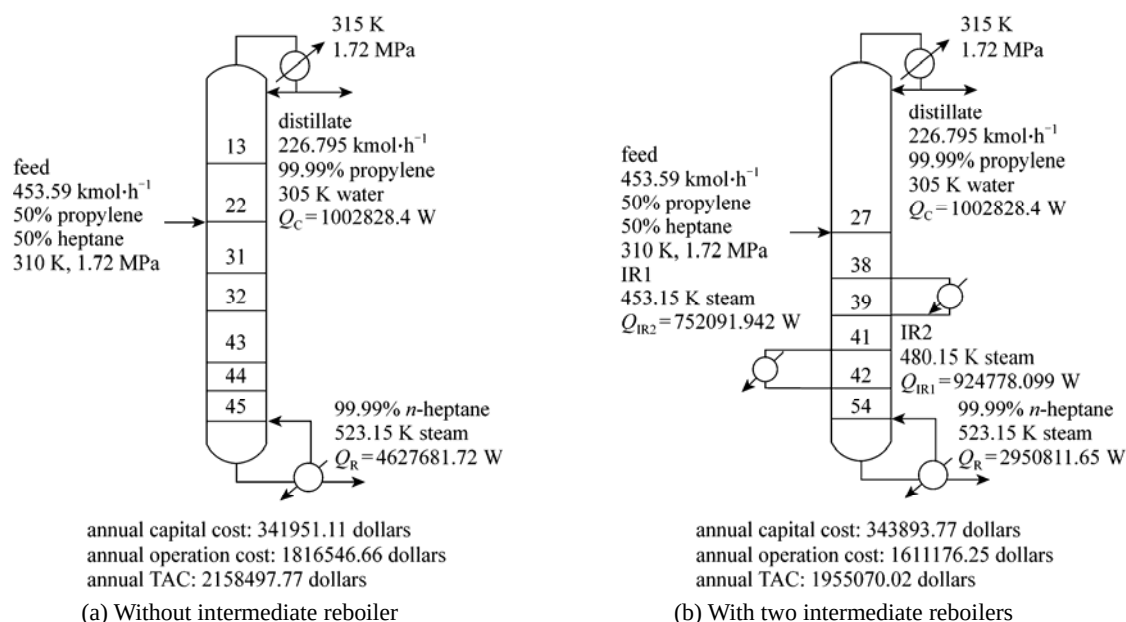


Figure 2 The optimal results for Example 1

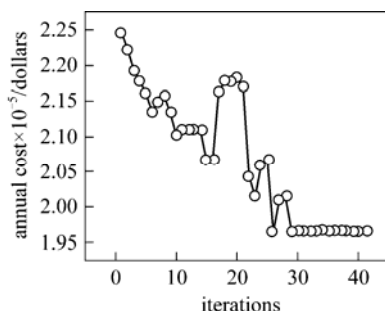


Figure 3 Converging course of annealing calculation

report was based on simulation where the commercial software Aspen Plus was used for design. The main design considerations made in this published report were to determine the optimum heat removal in the intermediate reboiler, by restricting only one intermediate reboiler arrangement with a specified placement location. To make a comparison between the proposed algorithmic approach and a simulation method as that suggested by Luyben, a synthesis problem considering only one intermediate reboiler structure is solved using the approach. To achieve this, the design is modified accordingly by adopting the same design considerations, the main cost data and the same utilities conditions as that was done in Luyben. With such modifications, the synthesis problem in this phase can be realized to optimize only the locations of intermediate reboiler and the amount of intermediate heat exchanged. Both the optima obtained with one intermediate reboiler by using our approach and the results provided by Luyben are shown in Figs. 4 (a) and (b), respectively. Comparisons from Fig. 4 show that both the location of intermediate reboiler and the parameters obtained from the approach are identical approximately to that given by Luyben, which illustrate the reliability of the developed algorithmic approach. A complete comparison with results would be desir-

able. Such a comparison however is not attempted since the different strategy and design consideration were adopted in each approach. For example, this published report presented only two different utility steams (one is for base reboiler and the other for intermediate reboiler), and hence to investigate more saving with more intermediate reboilers for the separation problem is somewhat restricted.

6.2 Example 2

This example considers a five-component mixture separation and the problem data is given in Table 2. The utilities available are the same as that given in Example 1 (Table 2).

Table 2 Components and mole fractions of the feed of Example 2

Component	Mole fraction
A. C_2H_6 (ethane)	0.003
B. C_3H_8 (propane)	0.227
C. C_4H_{10} (<i>n</i> -butane)	0.37
D. C_5H_{12} (<i>n</i> -pentane)	0.35
E. C_6H_{14} (<i>n</i> -hexane)	0.05

Note: feed flow = $453.59 \text{ kmol} \cdot \text{h}^{-1}$; overhead product recovery: B 99%; bottom product recovery: C 99%.

By performing the presented synthesis algorithm, the optimal including both base column and column with intermediate heat exchanger are obtained. Details of column designs and the economics are listed in Table 3. Due to the low bubble point of overhead products, the column needs to be operated at low temperature and the highest cooling medium must be used (Ammonia 1). In the optimum, one intermediate condenser is favored to be placed in stage 24 so that the cheaper water can be used as its cooling medium

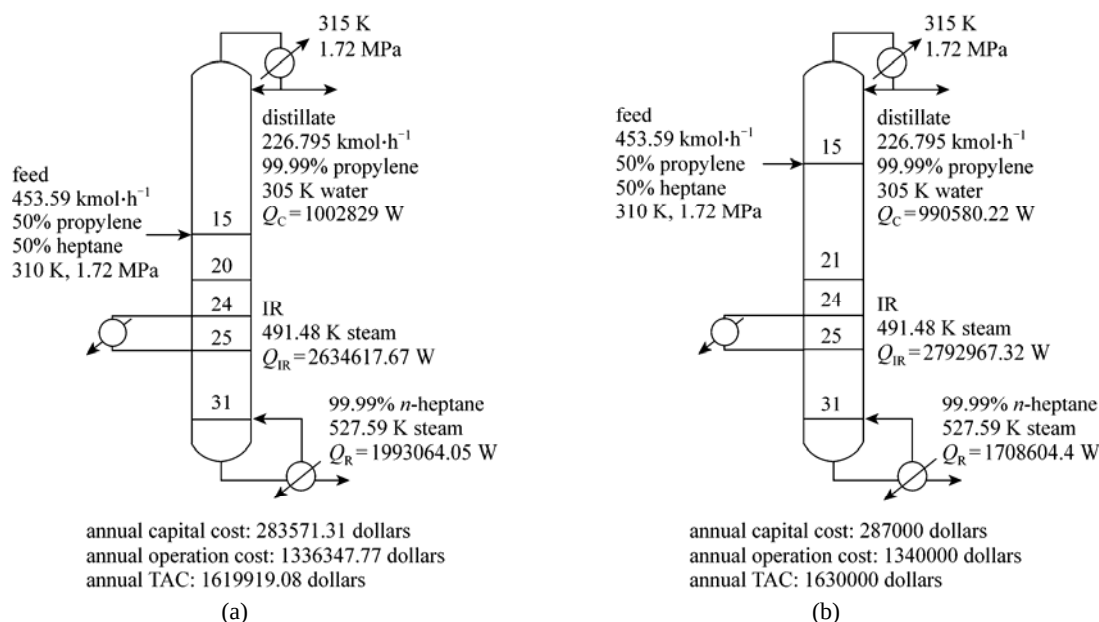


Figure 4 The comparison configurations between the algorithm (a) and literature (b)

Table 3 Comparing results of base column and column with an intermediate condenser

Equipment duty	Column without intermediate condenser	Column with an intermediate condenser
reflux ratio	3.985	3.985
pressure/kPa	456	456
number of stages	41	49
feed stage	28	35
location of intermediate condenser		24
condenser duty/ $\times 10^{-6}/\text{J}\cdot\text{s}^{-1}$	2.4722	1.1065
intermediate condenser duty/ $\times 10^{-6}/\text{J}\cdot\text{s}^{-1}$		1.3657
reboiler duty/ $\times 10^{-6}/\text{J}\cdot\text{s}^{-1}$	3.3850	3.3850
diameter/m	1.294	1.181
annual total capital cost/dollars	51048.58	59887.92
annual operating cost/dollars	180991.01	133298.92
annual total cost/dollars	232039.64	193186.84

instead of the highest cooling medium. Therefore, intermediate condensers can be used to reduce the operation cost of the column. From the results given in Table 2, by adopting an intermediate condenser, the total capital cost increases about 17.3%, but operating cost reduces about 26.3%. A saving of total annual is expected up to about 16.7% in comparison with an optimal conventional column, which shows the importance of adopting intermediate heat exchanger scheme for such a distillation problem.

7 CONCLUSIONS

This article proposes a SA-based strategy for the optimal synthesis of distillation column considering intermediate heat exchanger arrangements. Particular attention is made to develop an effective code-based procedure for structure representation so that the synthesis problem can be formulated as an MINLP form, to which an improved SA algorithm can be applied. The advantage of the approach is that the use of rules of thumb and on an exhaustive enumeration of all the possibilities can be avoided, which helps providing a rapid screening of alternatives for preliminary designs. The example studied shows that the developed approach was effective for the addressed problem. Also, the results demonstrate the economic importance of adopting intermediate heat exchanger scheme for different separation problems.

It should be pointed out that the illustrated cases in this article are just for obtaining an initial and based case to exam for a stochastic algorithm. Therefore the results obtained are only tentative, since a number of factors influence the economic performance of distillation with intermediate heat exchanger (*e.g.* boiling points, distribution of relative volatility and feed, utilities levels and prices, *etc.*). More efforts are worth to investigate for which effects are dominant and what mixtures the type of configuration yields the largest potential savings.

NOMENCLATURE

H	integer representing a search step-length
IC	intermediate condenser
IR	intermediate reboiler
L	integer representing a search step-length
M_C	match structure in rectifying section
M_H	match structure in stripping section
N_C	number of cooling mediums
N_H	number of heating mediums
N_r	number of stages in rectifying section
N_s	number of stages in stripping section
p	operating pressure of column
q_{IC}	heat duty of intermediate condensers
q_{IR}	heat duty of intermediate reboilers
r	pseudo-random number distributed between 0 and 1
U_C	number of cooling mediums
U_H	set of heating mediums
X	integer representing intermediate condenser structure
Y	integer representing intermediate reboiler structure
$\{\beta_j\}$	binary sequence for integer Y
$\{\phi_i\}$	binary sequence for integer X

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