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EXERGETIC OPTIMIZATION OF DISTILLATION SEQUENCES USING A GENETIC BASED ALGORITHM

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Abstract: Distillation is the most commonly applied method of separating multicomponent mixtures. Distillation systems are highly energy intensive and always consume a large amount of energy to achieve the objective. In a computer-based optimization, many alternatives of distillation sequences may be examined by varying the values of related integer variables. In the present study, an algorithm that is a hybrid of Nonlinear Simplex and a genetic algorithm that is a stochastic method based on the stochastic generation of solution vectors was used to minimize the sum of the annual capital and exergetic cost of the alternative sequences. The results of the example cases show that the proposed algorithm is applicable for the determination the optimum alternative of the distillation sequences.
Keywords: Distillation sequences, Genetic algorithms, Exergetic costing.

DESTİLASYON DİZİLERİNİN GENETİK TABANLI BİR ALGORİTMA İLE EKSERJETİK OPTİMİZASYONU

Özet: ZETÇok bileşenli karışımları ayırmada kullanılan en yaygın yöntemlerden biri olan destilasyon sistemleri, bu amaca ulaşmak için büyük miktarlarda enerji tüketirler. Bilgisayar desteğinde gerçekleştirilen destilasyon dizilerinin optimizasyonunda, destilasyon dizilerinin tüm alternatifleri, bu alternatifleri belirleyen tamsayılar vektörünün elemanları değiştirilerek irdelenebilir. Yapılan bu çalışmada, Doğrusal Olmayan Simplex ve rastgele sayıların kullanımına dayalı stokastik yöntemlerden biri olan, Genetik algoritmaların melezlenmesi ile oluşturulan, bir algoritma kullanılarak, destilasyon dizilerinin alternatifleri içerisinde yıllık bazda minimum ekserjetik maliyete sahip olan dizinin belirlenebileceği saptanmıştır. İncelenen örneklerin sonuçları, algoritmanın ve bu algoritma kullanılarak gerçekleştirilen yazılımın destilasyon dizilerinin alternatifleri arasından optimum olanının belirlenmesinde kullanılabileceğini göstermiştir.
Anahtar Kelimeler: Destilasyon dizileri, Genetik algoritmalar, Ekserjetik maliyet.

NOMENCLATURE

A_C	Heat transfer area for a condenser (m^2)
A_R	Heat transfer area for a reboiler (m^2)
B_F	Bottom flowrate (kmol/h)
C	Column
C_{column}	Installed capital cost for a distillation column ($)
C_{Cond}	Capital cost for a condenser ($)
C_{Reb}	Capital cost for a reboiler ($)
C_{Tray}	Installed capital cost for trays ($)
$C_{p,W}$	Heat capacity of water (kJ/kg °C)
$C_{\Delta Ex}$	Annual exergy destruction cost ($)
Cc_w	Annual cost of cooling medium ($)
c_w	Cost of coolant ($/kg)
D_c	The column diameter (m)
D_F	The flowrate of the distillate (kmol/h)
ExW	Exergy rates of the outlet of cooling water(MW)
ExS_i	Exergy rates of the steam inlet (MW)
ExS_o	Exergy rates of the steam outlet (MW)
ExF	Exergy rate of the feed stream (MW)
ExT	Exergy rates for top streams (MW)
ExB	Exergy rates for bottom streams (MW)
F_c	Cost index for columns
F_v	Vapour flowrate of the condenser inlet (kmol/h)
H_{bottom}	Enthalpy of bottoms (kJ/kmol)
H_c	Height of distillation column (m)
H_{feed}	Enthalpy of feed, (kJ/kmol)
H_{top}	Enthalpy of distillate (kJ/kmol)
M_F	Flowrate of feed (kmol/h)
M&S	Marshall and Swift index
NC	Number of components
NS	Number of the distillation sequence
P	Pressure (bar or atm)
P_c	Probability value of crossover
P_G	Probability value of new generation
P_M	Probability value of mutation
P_R	robability value of recombination
Pr	Problem sequence number
Q_C	Rate of heat flow for condenser (kJ/h)

Q_H	Rate of heat flow for reboiler (kJ/h)
R	Reflux ratio
TCC	Total annual cost of a column ($)
TAC	Total annual cost of the distillation sequence($)
$T_{c,in}$	Inlet temperature of cooling medium (K)
$T_{c,out}$	Outlet temperature of cooling medium (K)
T_D	Temperature of distillate (K)
T_F	Feed temperature of the column (K)
t_L	Life time (h)
U_C	Heat transfer coefficient for condenser (kw/m^2.°C)
U_R	Heat transfer coefficient for reboiler (kw/m^2.°C)
W_C	Flowrate of cooling water (kg/h)
W_s	Flowrate of steam (kg/h)

Greek Letters

ΔH_v	Latent heat of vaporization (kJ/kmol)
ΔT_{min}	Minimum allowable temperature difference for the reboiler (°C)
λ_{top}	Latent heat of vapour stream for condenser inlet (kJ/kmol)
λ_S	Latent heat of steam (kJ/kmol)
η	Tray efficiency

INTRODUCTION

The synthesis of distillation sequences is an important task in the synthesis of the total chemical processes. The synthesis of distillation sequences must be rigorously tackled, because these processes are important energy consumers and they require large investments in their equipments.

Sharp distillation indicates the separation of a mixture to almost pure products. In other words, the residual compositions can be neglected and the number of possible separation sequences increase markedly with the number of feed components. It is desirable to have a computer implementable procedure to determine a set of good sequences according to a given criterion. The problem of automatic synthesis of separation sequences can be defined as follows: given a feed stream in a known state, to synthesis a process systematically that isolates the specified product and the goal is to minimize the annualized cost of the equipments considering the thermal and exergetic behaviours.

Exergy is the maximum theoretical useful work (shaft work or electrical work) obtainable from a thermal system as it is brought into thermodynamic equilibrium with the environment while interacting with the environment only. Exergy is a measure of the departure of the state of the system from the state of the environment. The environment is a large equilibrium system in which the state variables (T_0, P_0) and the chemical components contained in it remain constant, when, in a thermodynamic process, heat and materials are exchanged between another system and the environment. No chemical reactions can take place among the environmental chemical components. The environment is free of irreversibility. The exergy of the environment is equal to zero. The laws of conservation of mass and energy state that the total mass and total energy can neither be created nor destroyed in a process. Exergy is not generally conserved but destroyed by irreversibility within a system. Exergy is being lost, in general, when the energy associated with a material or energy stream is rejected to the environment. The real thermodynamic inefficiencies in a thermal system are related to exergy destruction and exergy loss.

In the field of the synthesis of sharp separation sequences, a basic assumption has been made in all of the previous works: Each separator splits its feed mixture into two product streams; each component in the feed exists in only one of these streams. Because of this assumption, the number of alternatives of the sharp distillation systems depend on the number of compounds in the mixture separated. The number of such sequences, NS is given by:

$$NS = \frac{(2(NC-1))\,!}{NC!\;(NC-1)!} \qquad (1)$$

Determination of the optimum configuration: Kefeng et al. modelled the problem as a MINLP problem and proposed an improved genetic algorithm to determine the optimum configuration [1]. In that algorithm, each alternative was represented by 2n-1 dimensional arrays. Özçelik et al. modelled the problem as an integer programming problem and proposed a Branch and Bound algorithm for the solution of the model (Özçelik et al., 1999). In that algorithm, each configuration was represented by n-1 dimensional arrays.

In this study, the sum of equipment cost, utility cost and the exergetic cost of the configurations were minimized, for the first time, by using a different genetic based hybrid algorithm.

THE ALGORITHM AND THE COMPUTER PROGRAM

In this study, the algorithm and the computer program package were self developed using VB 6.0 to determine the optimum among the alternative distillation sequences based on exergy destruction. The flowchart of the algorithm is given in Figure 1.

The required data are provided by a database and the user. The database developed by Access-1997 includes the required constants of 550 pure compounds to calculate the physical properties of the pure compounds or mixtures for the given feed conditions.

The computer program developed using VB 6.0 involves the following three basic modules:

- The module that involves the functions to estimate the physical properties of the mixtures for the selected compounds for the given compositions. This module was developed to estimate the required physical properties of the streams of the distillation columns in the configuration.

- The module that involves the functions of the genetic based algorithm (Özçelik, 2007) to generate the values of the required discrete and continuous design parameters of the problem and to determine the optimum ones.
- The module that involves the functions to design and calculate the annual cost of distillation columns in the sequences and exergetic destruction for all determined alternatives of the distillation configuration.

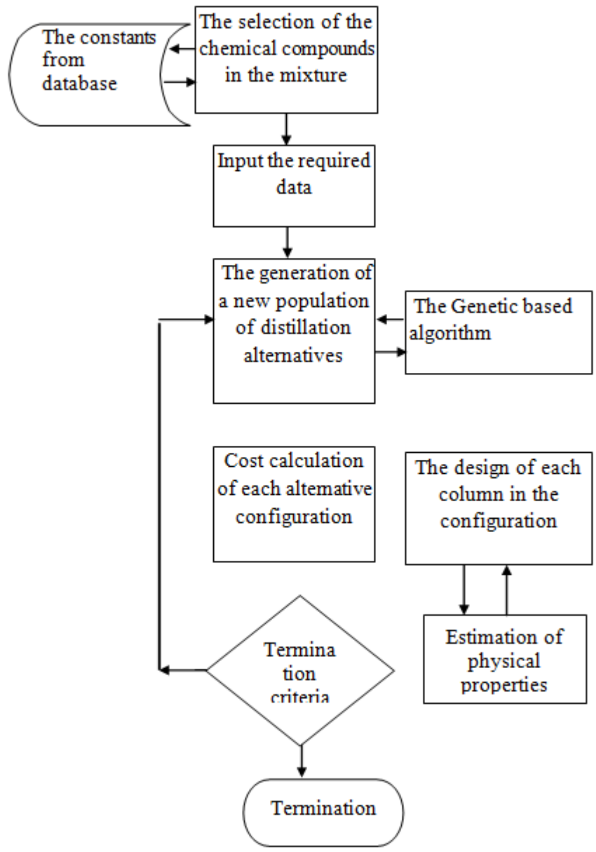

Figure 1. The flowchart of the algorithm.

The Genetic Based Algorithm

In this study, a hybrid algorithm based on the general principles of GA's and Nonlinear Simplex (Nelder and Mead, 1965) was used to search for the optimum values of continuous and discrete design parameters of the problem that are generated randomly using the following relationships.

$$x_{i+1} = x_i + r v_{mh} e_h \qquad (2)$$
$$y = LB + INT\,(u \times sr + 0.5) \qquad (3)$$

where x_i is the current optimum for the continuous variables. r shows the random numbers in the interval of [-0.5, 0.5] and u is the integer variable that can be either 0 or 1. e_h is the vector of the h^{th} coordinate direction and v_{mh} is the component of the step vector (v_m) along the same direction. LB and sr are the vectors of the lower bounds and the search region for discrete variables respectively. The values of the components of v_m were determined as 2.5 using the test functions taken from literature (Kefeng et al., 1998). The value of sr was taken as 1 to generate only 0 and 1 values by using the relations 2 and 3.

The discrete variables were used to determine the alternative distillation sequences in the strategy (Kefeng et al., 1998) that is described as follows. This was based on four components of the feed stream;

- The components are ordered based on increasing relative volatilities.
- (n -1) different integers are generated to represent decomposition points. The decomposition points (Kefeng et al., 1998) for a 4-component-mixture are shown in Figure 2.
- Each (n-1) dimensional array involving sequence number of decomposition points represents an alternative distillation sequence for n-component feed stream. Additionally, n-1 continuous variables determine the reflux ratios of the columns in the configuration.

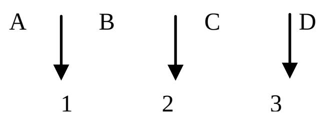

Figure 2. Decomposition points for a 4 – component-mixture.

Two possible arrays of integers that determine the decomposition points and alternative distillation sequences for these decomposition points are illustrated in Figure 3.

The basic steps of the genetic based algorithm (Özçelik, 2007) are given as follows:

- Encoding and initial population
  The algorithm uses real value encoding and the initial population, consisting of points in the feasible search space, is randomly created with a particular population size that is chosen as 10xN where N is the number of the variables.
- The generation of a new population
  Each new population is formed by applying the following operators:

1. Reproduction: Reproduction is the first operator applied on a population and the strings that have the best fitting values are picked from the current population and duplicates of them are inserted in the mating pool (elitist strategy).
2. Crossover: In the algorithm, the single point crossover is preferred and the strings are cut randomly and

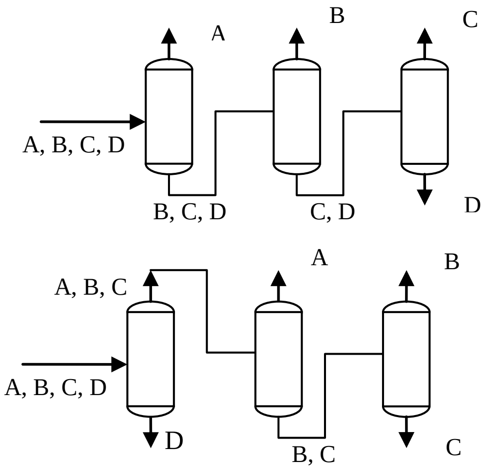

Figure 3. The distillation sequence alternatives of the 4-component-mixture (for the array of 1, 2, 3 and 3, 1, 2).

the right side portion of both strings swaps among themselves to create the binary variables of the new strings. The continuous variables of the new strings are created by applying the following crossover operators [1].

$$x_{offspring_1} = \frac{1-t}{2} x_1 + \frac{1+t}{2} x_2 \tag{4}$$

$$x_{offspring_2} = \frac{1+t}{2} x_1 + \frac{1-t}{2} x_2 \tag{5}$$

where t is a real number between 0 and 1. The value of t was calculated as 0.2 by using the test functions taken from literature [1].

3. Mutation: The position of the strings is determined randomly and a mutation operator is applied for that position. If the variable at the determined position is binary, it was changed depending on the current value. Otherwise, the continuous variables were replaced by the value at the same position of the different strings that are determined randomly in the current population.
4. Generation of new random vectors:Although the generation of new random vectors in each new population is not the general operator of the GA’s, it is used and the probability value is determined experimentally. In this step, the reflection and expansion functions of the nonlinear simplex algorithm (Nelder and Mead, 1965) are applied to the strings that have the same discrete values for the treatment of the continuous variables of the problem.

The proposed values of the percentages of reproduction, crossover, mutation and generation are given in Table 1.

Table 1. The probability values of the operators of the genetic based algorithm

P_R	P_C	P_M	P_G
30	40	5	25

- Termination criteria
  GA’s do not guarantee convergence to a global optimum solution hence a suitable stopping criterion is required. The constant number of generations or different termination criteria can be used to terminate the GA’s. In the present algorithm, the following termination criterion was used.

$$abs(F_{Avg_i} - F_{Avg_{i-25}}) \le \in \tag{6}$$

F_{Avg_i} and $F_{Avg_{i-25}}$ are the average objective function values for 25 consecutive generations.

Model description of the distillation column

Once the distillation tasks and their connection in distillation sequences have been determined, it is still necessary to specify the number of columns performing each distillation task and their operation conditions. The important operating variables in each column are the reflux ratio, the “feed vapour / liquid ratio”, and the column pressure. If the feed conditions, design pressures, reflux ratio, and the quality of the products are given, the capital and operating costs of the columns in the sequences can be determined. To calculate the cost of the column, it is necessary to calculate the diameter, height, and minimum number of trays in the columns (Pibouleau et al., 1983). The diameter (D_c) , minimum number of trays (N_{min}) and the height of the column (H_c) are calculated as follows:

$$D_c = \left\{ \frac{4}{\pi} D_F (R+1) \frac{22.2 T_D}{0.761(1/P)^{0.5}\, 273} \frac{1}{3600P} \right\}^{0.5} \tag{7}$$

$$N_{min} = \frac{\ln\left[\dfrac{n_{LK,D}}{n_{HK,D}} \dfrac{n_{HK,B}}{n_{LK,B}}\right]}{\ln \alpha_{LK-HK}} \tag{8}$$

$$H_c = 0.61 \frac{N}{\eta} + 4.27 \tag{9}$$

where n is the molar flow rate of the light key (LK) or heavy key (HK) in the related stream and α is the relative volatility of LK and HK. The last step consists of making a heat balance to compute the temperature at the top and the bottom of the column, the condenser duty and the reboiler duty, by using a thermodynamic model appropriate for the nature of the components to be separated.

The loads of the condensers and reboilers can be calculated from the energy balance around the condenser and around the overall column. The equations used for these balances are:

$$Q_c = (R+1)\, D_F\, \lambda_{top} \tag{10}$$

$$Q_H = H_{bot} + H_{top} + Q_c - H_{feed} \tag{11}$$

After the calculation of the column height and diameter, Guthrie's correlations were used (Guthrie, 1969) to estimate the tower cost; the shell cost and the cost of the trays were added. Process pressure vessels are usually designed in accordance with the current ASME pressure vessel codes and they are cylindrical shells capped by two elliptical heads. Wall thickness was included in the pressure factors. The base cost represents pressure vessels fabricated in carbon steel to resist 4.5 atm internal pressures with average nozzles, man way and supports. Other factors can be used to adjust for other shell materials, and pressures up to 70 atm. Tray assemblies, packed beds, lining, and other internals are priced separately and added to the shell cost as required.

$$C_{column} = \left(\frac{M\&S}{280}\right) 101.9\ (D_c/0.3048)^{1.066} (H_c/0.3048)^{0.802} (2.18+F_c) \quad (12)$$

$$C_{tray} = \left(\frac{M\&S}{280}\right) 4.7 (D_c/0.3048)^{1.55} (1.64NT) F_c \quad (13)$$

For a distillation column, the auxiliary equipments such as the condenser and the reboiler must be designed. Generally a total condenser is considered. Then the condenser heat duty is the heat required to completely condense the vapour passing overhead.

$$\begin{aligned} Q_c &= \lambda_{top} F_v = f(U_c, A_c, T_D, T_{c,i}\, T_{c,o}) \\ &= W_C C_{p_W} (T_{c,o} - T_{c,i}) \end{aligned} \quad (14)$$

An overall heat transfer coefficient for the condenser is assumed as $U_c = 2020$ kJ/m^2.h.K, it gives reasonable results (Özçelik et al., 1999) or a user defined value may be used. Hence, the required heat transfer area for the condenser and the required flow of the cooling water or refrigerated water are,

$$A_C = f(Q_c, U_c, \Delta T_{ln}) \quad (15)$$

$$W_C = f(Q_c, T_{c,i}, T_{c,o}) \quad (16)$$

The annual cost of the cooling medium is

$$C_{CW} = f(c_w, W_C) \quad (17)$$

If steam is used to supply the heat to produce V' (kmol/h) of vapour at the bottom of the tower, a heat balance gives the Q_H value around the overall column. At the same time,

$$Q_H = U_R A_R \Delta T_{min} = W_S \lambda_S \quad (18)$$

The temperature driving force in the reboiler must be constrained to be less than 0 to 7^{o}C, to prevent film boiling. There will be a limiting heat flux in the reboiler and a $U_R \Delta T_{min}$ value is assumed as 127754.16 (kJ/hr-K) (Douglas, 1988) or may be used a user defined value. The required heat transfer area and the steam supply are given by the following functions:

$$A_R = f(Q_H, \lambda_s) \quad (19)$$

$$W_S = f(Q_H, \lambda_s) \quad (20)$$

Similarly, the capital costs of the condenser and the reboiler can be found by using Guthrie's correlation (Eq. 21), if the range of the transfer area is between 10 m^2 and 1000 m^2.

$$C_{C-R} = 4936.8 A^{0.65} F_c \quad (21)$$

The total annual cost of a distillation column is given as:

$$TCC = (C_{Column} + C_{Tray} + C_{Cond} + C_{Reb})/t_L \quad (22)$$

In this study, the total annual cost of a distillation sequence is given as the sum of the annual cost of the distillation columns and physical exergy destruction of the configuration.

$$TAC = \sum_{i=1}^{NC-1} TCC_i + C_{\Delta Ex} \quad (23)$$

Exergy values were calculated for streams involving single compounds and the feed stream of the first column. Because, the exergy destruction of the configuration can be calculated using the exergy values of these streams.

The reference temperature and the temperature of the cooling water are 25 ºC. Therefore the exergy values of the inlet streams of the cooling water were taken as 0. In the reboilers of the distillation columns, low pressure steam (P = 3 atm) was used and entropy values of the saturated steam and saturated liquid at 133.55 ºC were used in the calculations of the exergy values of the hot medium.

In all of the exergy calculations, only the physical components of the exergy values were considered and the chemical and mixing exergies were neglected.

The values of 5000 h, 5 yr and 5 x 10^{-5} \$/W were used as operational hours, life time, and unit exergy cost in the cases.

RESULTS AND DISCUSSION

In this study, a computer program that can estimate the optimum values of the discrete and continuous variables of the exergetic optimization of the distillation sequences was developed. For this purpose, a tested genetic based algorithm (Özçelik, 2007) was used to estimate the optimum values of the continuous and integer variables of the example cases.

The synthesis for the best flow sheet for a multi-component separation problem constitutes as a formidable task even for a different size problem. The number of alternative and feasible column sequences increase rapidly as the number of components in the mixture and the number of allowed separation methods increase.

The processes with 3, 5 and 6 components design cases were analyzed. The integer and continuous variables of the mathematical model determine the alternatives of the distillation sequences and reflux ratios of the columns respectively. The required data for these cases are given in Table 2. The compounds in the mixtures are taken as, (1) n-Pentane, (2) n-Hexane, (3) n-Heptane, (4) n-Octane, (5) n-Decane, (6) n-Nonane.

Table 2. Data for cases 1, 2 and 3.

Case	Compounds	M_F	Mol %	P (Atm)
1	2, 4, 5	600	30, 28, 42	1
2	1, 2, 3, 4, 5	600	20,20,20,20,20	1
3	1, 2, 3, 4, 5, 6	600	15,15,15,20,20,15	1

In the first case, the feed stream involves 3 components and there are 2 possible distillation sequences. Each sequence involves 2 distillation columns. The results of the optimum configuration are given in Table 3 and 4, respectively.

Table 3. Results of Case 1.

C	Feed	D_c	H_c	R
1	1, 2, 3	1.87	16.45	0.49
2	2, 3	2.20	21.37	0.88

Table 4. Exergy values of the streams for Case 1.

Column	ExF	ExT	ExB	ExS_i	ExS_o
1	1.44	0.17	----	1.78	-0.17
2	----	0.59	1.75	1.95	-0.19

The feed stream involves 5 components for the second case and there are 14 possible distillation sequences. Each sequence involves 4 distillation columns. The detailed results for the optimum configuration and the distillation columns in the optimum configuration are given in Table 5 and Table 6 respectively.

Table 5. The results for Case 2.

C	Feed	D_c	H_c	NT	R
1	1,2,3,4,5	1.77	31.80	36	1.24
2	2,3, 4,5	2.46	29.96	34	0.85
3	2,3	1.89	31.64	36	1.30
4	4,5	1.70	23.80	26	0.58

Table 6. Exergy values of the streams for Case 2.

C	ExF	ExT	ExB	ExS_i	ExS_o
1	0.70	0.02	----	1.39	-0.14
2	----	----	----	2.46	-0.24
3	----	0.11	0.23	1.27	-0.13
4	----	0.41	0.83	1.63	-0.16

In the final case, the feed stream involves 6 components and there are 42 possible distillation sequences. Each sequence involves 5 distillation columns. The screen that shows the optimum configuration are given in Figure 4.

The detailed results of the optimum configuration and the distillation columns in the optimum configuration are also given in Table 7 and Table 8 respectively.

In the first case the feed stream involves 3 components and there are only 2 alternative distillation sequences. TAC of each alternative was calculated manually and the selection of the optimum sequence and the other results of the algorithm were corrected easily.

But, the numbers of alternative sequences are 14 and 42 for case 2 and 3 respectively. Therefore, these cases are resolved using the results handled by the program as an element of the initial population. It was observed that the final results achieved by the program were the same for both runs.

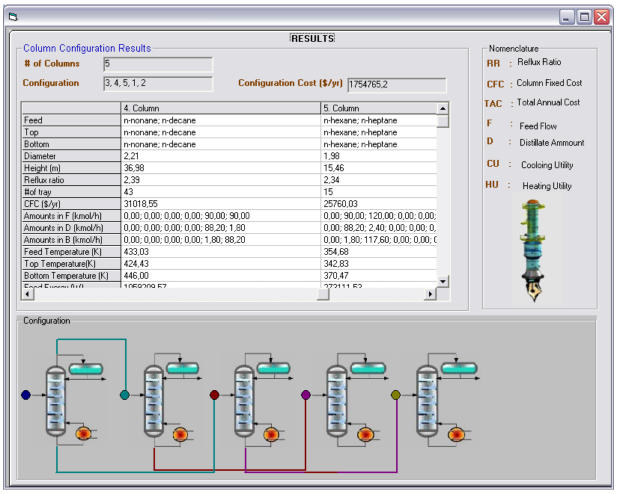

Figure 4. The optimum configuration for Case 3.

Table 7. The results for Case 3.

Column	Feed	D_c	H_c	NT	R
1	1,2,3,4,5	2.59	24.51	27	0.67
2	1,2,3	1.53	26.45	29	1.23
3	4,5,6	2.27	22.52	24	1.86
4	4,5	2.21	36.98	43	2.39
5	2,3	1.98	15.46	15	2.34

Table 8. Exergy values of the streams for Case 3.

Column	ExF	ExT	ExB	ExCW	ExS_i	ExS_o
1	0.88	----	----	4.31	2.93	-0.29
2	----	0.02	----	1.57	0.77	-0.08
3	----	0.40	----	3.52	2.61	-0.26
4	----	0.46	0.63	3.37	1.81	-0.18
5	----	0.08	0.23	2.64	1.43	-0.14

CONCLUSION

In this study, an algorithm and a computer program that can estimate the optimum values of the discrete and continuous variables of the exergetic optimization of the distillation sequences were proposed. To generate the possible alternative sequences and to estimate the values of the reflux ratios of the columns in the sequences, a tested genetic based algorithm was used.

Although there is no published study in the literature to determine the optimum design configuration based on the exergetic optimization, the test of the termination criteria by increasing the number of iteration results and the test of the cost of the alternative sequences for Case 1 show that the performance of the proposed algorithm can be considered and distillation sequences based on exergetic cost could be successfully determined.

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