

Optimal Distillation Sequencing Using a Genetic Algorithm

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Optimal distillation sequencing is a method for obtaining the best structure of multicomponent separation processes. Due to the significant contribution of the distillation sequences to the capital and operating costs for the whole chemical process, the development of a systematic framework that will select the optimal distillation sequences becomes an important research issue. Since distillation sequencing is a combinatorial problem, this paper elaborates an algorithm to handle the problem and explains how to employ a Genetic Algorithm (GA) to solve the problem. GA is an optimization technique imitating the biological process of natural selection (Darwin's rule) and natural genetics by which only the fit can survive. The distillation sequences were coded into the chromosome structure. A set of initial chromosomes was generated. The fitness values were computed considering all the constraints. The highest fitness values were given the highest probability to be selected in the next generation. The new population was generated by the processes of reproduction, which were duplication, cross linking and mutation. The effects of GA parameters such as the population size and the probabilities of reproduction, crossover, and mutation on the convergence rate were studied. Two cases, that is, 4-component and 5-component systems were employed to validate the developed program. The correct solutions were obtained. It was found that the population size should be kept close to the number of possible sequences. The study showed that there were optimal values for the cross link and mutation probabilities. For the case of the 4-component system, the optimal cross-link and mutation probabilities were in the ranges of 0.7-0.85 and 0.004-0.007, respectively.

Key words: Genetic Algorithm, distillation sequencing, optimization.

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การหาลำดับที่เหมาะสมที่สุดเป็นวิธีการกำหนดโครงสร้างที่ดีที่สุดสำหรับกระบวนการกลั่นแยกสารหลายองค์ประกอบ เนื่องลำดับการกลั่นเป็นปัจจัยที่ส่งผลกระทบต่อค่าใช้จ่ายในการลงทุนและในดำเนินกระบวนการอย่างมาก การพัฒนากรอบการจัดลำดับอย่างเป็นระบบจึงเป็นประเด็นสำคัญของการวิจัย เนื่องจากปัญหาการจัดลำดับการกลั่นเป็นปัญหา combinatorial บทความนี้นำเสนอขั้นตอนวิธีการคำนวณที่ใช้ในการแก้ปัญหาและอธิบายการนำขั้นตอนวิธีเชิงพันธุกรรมมาใช้ในการแก้ปัญหา ขั้นตอนวิธีเชิงพันธุกรรมเป็นเทคนิคการหาค่าที่เหมาะสมที่สุดซึ่งเลียนแบบกระบวนการทางชีวภาพในการคัดสรร (กฎของดาร์วิน) และการปฏิบัติการทางพันธุกรรมทางธรรมชาติ โดยผู้ที่เหมาะสมคือผู้ที่อยู่รอด ลำดับของการกลั่นถูกใส่รหัสในโครงสร้างโครโมโซม และมีการสร้างชุดของโครโมโซมเริ่มต้นเพื่อใช้ในการคำนวณ โดยทำการคำนวณค่าความเหมาะสมที่ผ่านข้อจำกัดต่างๆ ให้โครโมโซมที่มีค่าความเหมาะสมสูงสุดมีโอกาสสูงสุดที่จะได้รับเลือกเป็นตัวแทนสำหรับการคำนวณในรุ่นต่อไป ประชากรชุดใหม่ได้จากการทำโครโมโซมซ้ำ การไขว้โครโมโซมและการเปลี่ยนแปลงโครโมโซมใหม่ นอกจากนี้ยังได้ทำการศึกษาผลกระทบของพารามิเตอร์ในวิธีการพันธุกรรม เช่น ขนาดประชากร ความน่าจะเป็นในการทำโครโมโซมซ้ำ การไขว้โครโมโซม และการเปลี่ยนแปลงโครโมโซมใหม่ต่ออัตราเร็วในการพบคำตอบ ใช้กรณีศึกษา 2 กรณีในการแสดงความถูกต้องของโปรแกรมคอมพิวเตอร์ที่พัฒนาขึ้นจากการทดสอบพบว่าโปรแกรมทำงานถูกต้อง สำหรับการศึกษาค่าพารามิเตอร์พบว่าจำนวนประชากรของโครโมโซมควรมีจำนวนใกล้เคียงจำนวนขั้นลำดับที่เป็นไปได้ทั้งหมด โดยที่มีค่าความเหมาะสมค่าหนึ่งสำหรับค่าความน่าจะเป็นของการไขว้โครโมโซมและการเปลี่ยนแปลงโครโมโซมใหม่ สำหรับกรณีสารองค์ประกอบ 4 ชนิด ค่าความน่าจะเป็นสำหรับการไขว้โครโมโซมและการเปลี่ยนแปลงโครโมโซมใหม่อยู่ระหว่าง 0.6-0.9 และ 0.004-0.119 ตามลำดับ

คำสำคัญ การจัดลำดับการกลั่น วิธีเชิงพันธุกรรม การหาค่าที่เหมาะสม

INTRODUCTION

The distillation column is one of the most important unit operations in chemical processes. Normally, a train of the units will be used in order to separate the chemicals from a mixture. This brings up the issue of how the columns should be arranged, since different arrangements lead to different investment and operating costs. Therefore, for more than a decade chemical engineers have developed procedures for helping process designers to decide how to configure the process so that the total cost is minimal. Pibouleau and Domenech⁽¹⁾ developed discrete and continuous approaches to synthesize the optimal distillation sequencing. They first solved the discrete problem with integer programming (IP) using bound and branch algorithms and then solved the continuous problem with nonlinear programming with reduced gradient algorithms. Gadkari and Govind⁽²⁾ developed a procedure based on the volumetric flow between stages in the column to estimate the cost of the investment. The procedure was used together with a heuristic approach to find the optimal sequence. Wahl and Lien⁽³⁾ explained a mathematical technique with a so-called "generating function," which was used to describe the fundamentals of the equation for calculating all possible distillation sequences. Flowers and Harrison⁽⁴⁾ developed an automated distillation sequencing system (DSEQSYS), which is composed of three parts: a control program, fuzzy heuristic synthesis program, and simulation program. In that year, Floquet et al.⁽⁵⁾ also developed a fuzzy heuristic approach for sharp sequence synthesis. Regarding to the application of genetic algorithms (GA), Androulakis and Venkatasubramanian⁽⁶⁾ applied GA to optimize a heat exchanger network and Manolas et al.⁽⁷⁾ also applied GA to optimize a cogeneration system by studying the effects of

the population size and probability of the mutation. McKay, Willis, and Barton⁽⁸⁾ applied GA for modeling of chemical process systems. Garrard and Fraga⁽⁹⁾ applied GA for synthesizing the mass exchange network.

The purpose of this paper is to demonstrate how to apply GA to solve problems of distillation sequencing and how GA parameters affect the solution of the problem. It was assumed that the separation was the sharp-split.

Problem Formulation

The formulation used in this paper is similar to that of Andrecovich and Westerberg.⁽¹⁰⁾ The problem was formulated as MILP (Mixed Integer Linear Programming). The objective function can be written as:

Minimize

$$P(I_k, y_k, S_k, F_k, C_H, C_C, Q_k) \\ = \sum_{k \in COL} [I_k y_k + S_k F_k + (C_H + C_C) Q_k] \dots (1)$$

Here P is the cost function of the selected configuration. It comprises the costs due to the capital investment and operating costs. The capital investment is a function of the types of columns used in the configuration, y_k , the sizes of the columns, S_k , and the amount of feed, F_k . Also, I_k is a binary variable which has a value of zero or one. It indicates whether the column is in the selected configuration. The operating costs include the costs due to the duty of heating, C_H , and that of cooling, C_C , used in the process, assuming that the sum of both of the duties is equal to Q_k . From the objective function above, it is clear that the expression is a mixture of integer and real variables.

The constraints comprise both equality and inequality constraints. The equality constraints are the material balances, Equations (2) and (3) and energy balances, Equation (4). The first equation is for the column that has the feed as the initial mixture. The other expresses material balance among the columns for separating intermediates. The constraints can be written as:

$$\sum_{k \in FS_F} F_k = F_{TOT} \quad \dots(2)$$

and

$$\sum_{k \in FS_m} F_k - \sum_{k \in PS_m} \xi_k^m F_k = 0 \text{ for } m \in IP \quad \dots(3)$$

where FS_F , FS_m , and PS_m are the sets of columns k that have as feed the initial mixture, as feed the intermediate m , and as product the intermediate m , respectively. The set IP is the set of intermediate products. Then,

$$Q_k - K_k F_k = 0 \quad k \in COL \quad \dots(4)$$

$$F_k - U y_k < 0 \quad k \in COL \quad \dots(5)$$

$$F_k, Q_k \geq 0 \quad k \in COL \quad \dots(6)$$

$$Y_k = 0, 1. \quad k \in COL \quad \dots(7)$$

Equation (4) represents the energy use in each column, where Q_k values are the heat duties of condensers and reboilers and K_k values are the heat duty coefficients for each column. It is assumed that the duty requirement for each column is proportional to its feed rate. Also, U is the upper limit of the feed rates. The y_k values are binary variables, and COL represents a column in the superstructure.

Genetic Algorithms

GAs⁽¹¹⁾ are search algorithms based on the mechanics of natural selection and natural genetics. This implies that the process will involve randomized processes. The information from the problem will be converted into string structures. These structures imitate the chromosomes of living cells. These structures will be evaluated for their fitness. The ones that have higher fitness values will have higher survival rates. The process of finding an optimum point is carried out as an iterative approach. It exploits the historical information to project new search points with expected improved performance. In each generation, a new set of chromosomes is generated using bits and pieces of the fittest of the old; an occasional new part is formulated for good measure.

GAs were developed by John Holland in 1975 with two objectives: first, to abstract and rigorously explain the adaptive processes of natural systems and second, to design artificial systems software that retains the important mechanisms of the natural systems. The method is a search procedure that uses random choice as a tool to guide a highly exploitative search through a coding of a parameter space. From their research, they have concluded that GAs are theoretically and empirically able to provide robust searches in complex spaces. The algorithms are computationally simple and powerful. Furthermore, the methods set no limitations or restrictive assumptions on the search spaces, such as continuity, existence of derivatives, or unimodality. Recently, researchers have recognized the shortcomings of calculus-based and enumerative optimization techniques, since they have a number of limitations and are not robust. Therefore, the random search algorithms have achieved increasing popularity.

GAs are different from conventional optimization methods and search procedures in the following ways: a) GAs work with a coding of the parameter set, not the parameters themselves. b) They search from a population of points, not a single point; c) They only use knowledge of the objective function or performance function. d) They use probabilistic rules, not deterministic rules. According to item (a), finite-length alphabetic strings imitating natural chromosomes will be exploited to represent the parameter set of the optimization problem. Quite often, a binary number is used for each character in the string. However, it is not necessary that each character has to be binary. GAs simultaneously work with a database of feasible solutions, searching many peaks in parallel; the probability of finding a false peak is reduced over methods that go from point to point. GAs do not need auxiliary information to work properly. They only need the objective function values associated with individual strings. Although the methods use probabilistic rules to search for a new solution, it is not a simple random search. The probabilistic rules are used as a tool for increasing the opportunity for a better solution to be selected in the next generation. With this mechanism, the population will most likely have better members than the previous generation. This is the way in which a GA guides the search toward improved regions of space.

A simple GA is composed of three operations: reproduction, crossover, and mutation. Reproduction is the process in which a string in the population in the previous generation is copied to become one in the next generation. On the other hand, crossover is the process in which strings in the population are mating. A new string is created by swapping characters from certain

positions in one string with those in the other string. Thus the crossover involves partial string exchanges. The last operation is mutation. It is needed since occasionally reproduction and crossover operators become overzealous and lose some potentially useful genetic material. The mutation operator protects against such irrecoverable loss. The mutation is an occasional random alteration of the value of a string position. The alteration takes place with a very small probability.

Chromosome Definition

The chromosomes or the character strings are used to carry the values of the parameters of the problem in GAs. For the distillation sequencing problem, the parameters are the types of columns that will be selected for the separation operation. This paper proposes that the length of chromosomes be the same as all possible columns in the superstructure or the number of possible columns or unique splits.⁽¹²⁾ Binary values are used for genes in the chromosome.

Performance Evaluation

The mechanism of selecting the members from a population for survival to the next generation mainly relies on the performance evaluation. In this paper the objective function in equation (1) is used as the performance function. The chromosomes with the lowest performance function values will have the highest fitness values. The roulette wheel analogy is used for the selection. The chromosomes with higher fitness values occupy more space on the wheel. Therefore, they will have a greater opportunity to be selected and a higher probability to be members in the next generation.

Figure 1. Flow diagram for finding feasible chromosomes.

Figure 2. Flow diagram for an optimization process using a GA.

Genetic Operations

The new chromosomes were obtained by using three kinds of genetic operations: reproduction, crossover, and mutation. Reproduction is the main operation. However, crossover and mutation also took place with certain probabilities, P_c and P_m , respectively. The probabilities of these operations were specified. This paper selects to allow the crossover to take place at only one position. The position was picked randomly. Every bit in the chromosome could be mutated. If the number drawn from a random number generator for a certain bit has a value higher than the probability of mutation, that bit will be changed; otherwise it will be the same.

Method of Calculation

Since separation sequencing is a combinatorial problem,⁽¹³⁾ the number of columns involved in the calculation can be increased rapidly when the number of components in the mixture is increased. Therefore, the method to handle the superstructure of the column sequence will be very important. In this paper, it was proposed to store the structure and feed information as follows: Four variables, "Subgroup," "Substr," "Product," and "FlowrateSub" were used to store the information. The "Subgroup" variable is a one-dimensional array that holds the information of all possible feed components. Its dimension is equal to $L = G - R$ where G is the number of subgroups and R is the number of components in the system. Each variable uses a link-list data structure type to store information of the component in each variable. The "Substr" variable is also one-dimensional array that holds the information of feed components to all possible columns. The size of its dimension is equal to the number of unique splits. The "Product" variable is a two-dimensional array. The first index indicates the type of column and

its size will be equal to the number of unique splits. The other indicates the products of that column with two possible values for this index. The last array stores the value of the feed rate for each column. The size of the array is the same as that of "Subgroup." With this data structure, the number of variables in the system will not drastically increase with an increase in the number of components.

The procedure was started by randomly generating a set of chromosomes, S . Then, each chromosome would be checked as to whether its conditions complied with all constraints, especially equations (2) and (3). Figure 1 shows the flow diagram of the program that was developed for checking the feasibility of the chromosomes. If a generated chromosome complied with the constraints, it would be selected to be a candidate in the population and the process would be carried out until all candidates were recruited. If the generated chromosome violated the constraints, it would not be chosen as a candidate, and a new chromosome would be randomly generated.

After obtaining the chromosome population, each chromosome would be evaluated for its performance index by using equation (1) and given information from users to calculate the cost. The fitness value was then calculated by

$$fitness = \frac{maxcost - cost_i}{(S)(maxcost) - \sum cost_i}, \dots (8)$$

where *maxcost* is the maximum cost among chromosomes in that generation and *cost_i* is the cost of the sequence due to the *ith* chromosome. The fitness will be used in the process of chromosome selection as mentioned earlier. The genetic operations proceeded as shown in the flow diagram of

optimization by using the GA (Figure 2). Since a GA employs a stochastic optimization, the solution always contains some uncertainty. Thus, conventional convergence criteria cannot be directly applied to the solution. Instead of measuring the change of the solution, one of the approaches is to measure the change of the average of the solution in each generation. If the change is less than the specified tolerance, the solution is considered converged. The other approach is to set a maximum number of generations and let the program run until exceeding the limit. The results and statistical data will be analyzed and conclusions will be drawn. The code was written using the Pascal language. The program was run on a 166 MHz Pentium II computer. Two cases, 4- and 5-component separations, were run to validate the program and to compare the results with those in the literature.

RESULTS AND DISCUSSION

Application of Distillation Cases

To validate the proposed program for finding the optimal sequence of the distillation columns, two typical separation problems were chosen as case studies. The first case was the case of 4-component separation. The economic data were

adopted from Biegler et al.⁽¹³⁾ as shown in Table 1. The second case was the case of 5-component separation. The components are propane, isobutane, n-butane, isopentane, and n-pentane. The Peng-Robinson thermodynamic model was used in the simulations. However, the economic data for this case were not available. To construct the required data, the HYSYS program, Chemical Process Simulator, was run. All possible columns were sized. The energy consumption in each column was estimated. The results are shown in Table 2. The required data for the program were expressed for Cases 1 and 2. The numerical experiments were also conducted with varying genetic parameters, such as probabilities of crossover and mutation and the number of chromosomes in the population, in order to observe the effect on the solution and the convergence rate.

After running the program, it was found that the optimal sequences for both cases were the structures as shown in Figures 3 and 4 for 4-component and 5-component systems, respectively. The cost was \$3,308,000/yr for the 4-component system and \$1,445,000/yr for the 5-component system. The results were consistent with those in the literature.

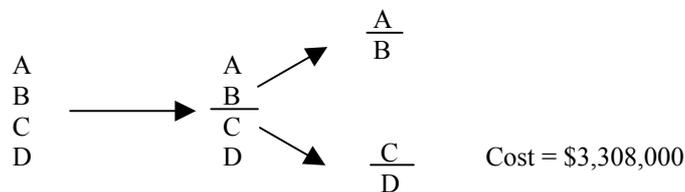


Figure 3. Optimal sequence for 4-component case.

Table 1. Economic data and heat duty coefficients.

Case 1. A 4-component separation process (Biegler et al., 1997)

Initial feed: $F_{TOT} = 1000$ kmol/hr

Composition: $A = 0.15, B = 0.30, C = 0.35, D = 0.2$

K	Separator	Investment cost		Heat duty coefficients K_k (10^6 kJ/kmol yr)
		Fixed cost I_k (10^3 \$/yr)	Variable cost F_k (10^3 \$hr/kmol yr)	
1	A/BCD	145	0.42	0.028
2	AB/CD	52	0.12	0.042
3	ABC/D	76	0.25	0.054
4	B/CD	38	0.14	0.040
5	BC/D	66	0.21	0.047
6	A/BC	125	0.78	0.024
7	AB/C	44	0.11	0.039
8	C/D	58	0.19	0.044
9	B/C	37	0.08	0.036
10	A/B	112	0.39	0.022

Cost of utilities: cooling water $C_C = 1.3$ (10^3 \$/ 10^6 kJ yr), Steam $C_H = 34$ (10^3 \$/ 10^6 kJ yr)

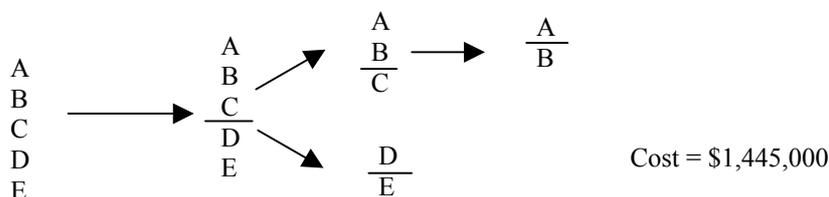


Figure 4. Optimal sequence for 5-component case.

Effects of Genetic Parameters and Population Size

The results obtained from studying the effects of genetic parameters are as follows (Figures 5-9): When the value of P_c was set to be one and P_m was set to 0, the algorithm quickly converged to a solution, but not the optimal one. The solution could not be improved any more as shown in Figure 5. Androlakis and Venkatasubramanian⁽⁶⁾ called this phenomenon "premature convergence." On the other hand, when the value of P_c was

set to be zero and P_m was set to 1, the solution behaved like a random variable. As observed in Figure 6, the solution oscillated and did not converge.⁽¹⁴⁾ suggested that one should select a high value for P_c , while P_m should be kept low. In this study, P_c and P_m were varied in order to observe the number of generations required in each case. Figure 10 shows that there were certain values of P_c and P_m which resulted in a minimum number of generations. However, these values are likely to vary from case to case.

Nevertheless, the ranges of P_c and P_m in this case were between 0.7 and 0.85 and between 0.004 and 0.007, respectively. The effect of the population size was also investigated. It was found that it affected the convergence rate in the sense that the rate was slower when the population was larger. Comparing Figures 7, 8 and 9, for population sizes of 6, 10, and 20, respectively, the generation that 5, 12, or 18, respectively. It was noted that the cases with a larger population size required a higher number of generations before

obtaining the optimal solution. However, the average solution oscillates less for larger population. It was also noticed that when the population size was smaller than the number of possible sequences, the solution had a high probability to be prematurely convergent. Therefore, in this study, it was concluded that the population size should not be too small. The selected size might be equal to the number of subgroups in the separation. For the 4-component system, the population size would be 10 and for the 5-component system the size would be 15.

Figure 5. Production cost of 4-component system with population size = 6, $P_c = 1$, and $P_m = 0$.

CONCLUSIONS

In conclusion, there are two points to be emphasized. First, a general computer code was developed to handle finding the optimal sequence of distillation columns for the mixture. Currently, the program was designed for a mixture of 10 components. However, the number of components can easily be changed. It also elaborated the procedure used to store the information of the superstructure of the separation process.

Second, it demonstrated how to find optimal distillation sequencing by using genetic algorithms. Two examples were used to validate the developed program. The effects of genetic parameters were also investigated. It was found that there were certain values of P_c and P_m that required the minimum number of genetic operations, and the size of the population could be the same as the number of subgroups.

Table 2. Economic data and heat duty coefficients.

Case 2. A 5-component separation process

Initial feed: $F_{TOT} = 360$ kmol/hr

Composition: $C_3 = 0.05, iC_4 = 0.15, nC_4 = 0.25, iC_5 = 0.20, nC_5 = 0.35$

K	Separator	Investment cost		Heat duty coefficients $K_k (10^6 \text{ kJ/kmol yr})$
		Fixed cost $I_k (10^3 \text{ \$/yr})$	Variable cost $F_k (10^3 \text{ \$ hr/kmol yr})$	
1	A/BCDE	1.4	0.086	0.007
2	AB/CDE	2.5	0.149	0.026
3	ABC/DE	1.6	0.095	0.021
4	ABCD/E	3.7	0.225	0.067
5	B/CDE	2.4	0.143	0.028
6	BC/DE	1.6	0.094	0.021
7	BCD/E	3.8	0.230	0.072
8	A/BCD	1.8	0.111	0.009
9	AB/CD	3.4	0.203	0.039
10	ABC/D	2.1	0.126	0.026
11	C/DE	1.6	0.098	0.021
12	CD/E	4.0	0.241	0.077
13	B/CD	3.0	0.199	0.040
14	BC/D	2.1	0.127	0.027
15	A/BC	2.3	0.141	0.011
16	AB/C	4.4	0.266	0.052
17	D/E	4.9	0.296	0.101
18	C/D	2.3	0.140	0.027
19	B/C	4.5	0.271	0.056
20	A/B	3.8	0.228	0.015

Cost of utilities: cooling water $C_C = 4.5 (10^3 \text{ \$/}10^6 \text{ kJ yr})$, steam $C_H = 30 (10^3 \text{ \$/}10^6 \text{ kJ yr})$

Figure 6. Production cost of 4-component system with population size = 6, $P_c = 0$, and $P_m = 1$.

Figure 7. Production cost of 4-component system with population size = 6, $P_c = 0.8$, and $P_m = 0.01$.

Figure 8. Production cost of 4-component system with population size = 10, $P_c = 0.8$, and $P_m = 0.01$.

Figure 9. Production cost of 4-component system with population size = 20, $P_c = 0.8$, and $P_m = 0.01$.

Figure 10. The response of the number of generations required for convergence the changes of probabilities of crossover and mutation.

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