Automated Synthesis of Distillation Sequences Using Fuzzy Logic and Simulation

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An automated distillation sequencing system (DSEQSYS) is presented, which consists of three components: a control program, a fuzzy heuristic synthesis program, and a process simulator. DSEQSYS, when applied to problems previously reported in the literature, overcomes some of the disadvantages of using heuristics or mathematical programming alone. DSEQSYS can address problems involving nonsharp separations, nonideal chemical behavior, and conflicting heuristics. A simple approach for converting the traditional separation heuristics into corresponding fuzzy heuristics is also demonstrated.

Introduction

Recent progress in process synthesis by no coincidence parallels developments in the fields of artificial intelligence and mathematical programming. The scope and complexity of these problems make them quite overwhelming without the aid of sophisticated computerized search techniques. The set of all possible orderings of a given separation task set describes the design space for distillation sequence synthesis. Those separations that are necessary to achieve the desired product set, compose the separation task set. For instance, consider the separation of a mixture into product streams by simple distillation. The number of distillation sequences, S_n, is related to the number of products, n, by the Eq. 1. Clearly, the number of possible sequences to consider becomes overwhelming as the number of products increases:

$$S_n = \frac{[2(n-1)]!}{n!\,(n-1)!} \tag{1}$$

Two approaches are evident: (1) consider the entire design space and select the optimal design; (2) reduce the design space until an acceptable design remains. The first approach is that of mathematical programming. The second is the more traditional one based on the use of heuristics. The automation of either such design process is possible.

Expert systems have been developed for the automation of the heuristic based synthesis by Kirkwood et al. (1988) and Crowe et al. (1992). However, expert systems are not capable of developing a guaranteed optimal design and may even miss good designs if heuristics conflict. This is because expert systems search for a single path to a goal. The first such path identified by the expert system represents the solution. Raman and Grossmann (1991) demonstrate that expert systems using either forward or backward chaining search techniques can miss solutions if heuristics conflict.

Therefore, it is necessary to identify and resolve heuristic conflicts during the design process to ensure the development of a good design. There are three points in the heuristic design process where conflict may arise. First, many of the heuristic based design techniques group heuristics into sets and require the designer to select the appropriate set. There may be multiple sets that are applicable. Secondly, conflict may arise between the heuristics within a given set. Finally, the heuristics may lead to multiple designs. It has been demonstrated by Huang and Fan (1988) that fuzzy logic provides a convenient method for resolving conflicts arising during heuristic set selection. The heuristic approach, unfortunately, provides no method for addressing nonlinear or nonideal behavior.

On the other hand, the mathematical programming approach addresses both nonlinear and nonideal behavior, and can provide optimal designs. These mathematical programs may consist of thousands of linear and nonlinear equations

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containing both discrete and continuous variables. Mathematical programming based design seeks to develop and optimize a superstructure of the design space. This necessarily restricts design considerations to the proposed superstructure. Therefore, the development of an automated design system, based on this approach, would require the specification of all such superstructures. Hence, the formulation of a mathematical program to solve a practical problem may require a substantial investment of time.

A practical solution may be possible by some intermediate combination of artificial intelligence, optimization, and rigorous process modeling. Diwekar et al. (1992) present one such hybrid approach, consisting of a MINLP (mixed integer nonlinear program) imbedded in the public version of ASPEN. Also, Raman and Grossmann (1991) have demonstrated that heuristics can be incorporated in mathematical programs. In this article, an automated system for distillation sequence synthesis (DSEQSYS) based on fuzzy heuristics and process simulation is presented, which generates a flowsheet for the sequence based only on the problem specifications.

Fuzzy Logic

The heuristics used for distillation sequence synthesis can conveniently be represented by fuzzy sets. Once developed, these fuzzy heuristics can then be used in the automation of distillation sequence synthesis. A high level of proficiency in fuzzy set theory is not requisite for the development of the heuristic sets. The heuristic sets used in this synthesis system are presented after a brief mathematical background is developed.

Mathematical preliminaries

Developments in the field of set theory by Zadeh (1964), led to what is known as fuzzy set theory. The concept of fuzzy sets is based on the idea of vagueness: sets without sharp boundaries. Fuzzy sets may also be based on probabilistic arguments, though they need not be. A relation or function defined on a given universe may be used to describe a fuzzy set. Consider a universe, U, and a fuzzy set, A, defined on U in Eq. 2:

$$A = \{[x, \mu_A(x)], x \in U\} \quad \mu_A(x) \in [0, 1] \tag{2}$$

The term $\mu_A(x)$ is the degree of membership in A that x possesses. Terms $\mu_A(x)$ will be referred to as descriptors. Therefore, a fuzzy set is composed of elements consisting of a pair, x and $\mu_A(x)$. If $\forall x \in U$, $\mu_A(x) = 0$ then $\mu_A(x)$ represents the empty set, $\varnothing$, and is denoted $\mu_\varnothing(x)$. For a fuzzy set, A if $\exists x \in U$, such that $\mu_A(x) = 1$, then A is said to be a normalized fuzzy set. Those elements $x \in U$ for which $\mu_A(x) = 1/2$ are known as the crossover points of A. The support of a fuzzy set, A, is defined as the set of all nonzero descriptors of A as shown in Eq. 3:

$$\operatorname{supp} A = \{x \in U, \mu_A(x) > 0\} \tag{3}$$

The union and intersection of two fuzzy sets, A, and B, are defined by Zadeh (1965) in the following way:

$$\forall x \in U, \ \mu_{A \cup B}(x) = \max[\mu_A(x), \mu_B(x)] \tag{4}$$

$$\forall x \in U, \ \mu_{A \cap B}(x) = \min[\mu_A(x), \mu_B(x)] \tag{5}$$

Zadeh (1965) also defined the compliment, $\overline{A}$, of a fuzzy set, A, as:

$$\forall x \in U, \ \mu_{\overline{A}}(x) = 1 - \mu_A(x) \tag{6}$$

In general, the intersection of a fuzzy set with its compliment is not empty as it is with traditional discrete sets. Subsets of a fuzzy set, A, which contain only those elements of A that are greater than some threshold value, say λ, are called the λ-cut of A, and are defined in Eq. 7:

$$A_\lambda = \{x \in U, \mu_A(x) \geq \lambda\} \quad \lambda \in (0, 1) \tag{7}$$

Dubois and Prade (1980) present an exhaustive research monograph that covers the majority of the work in this field before 1978.

Heuristic Representation. Consider the following list of heuristics:

- Eliminate forbidden separations
- Prefer easy separations
- Prefer equimolar separations

The adjectives describing the separations are the essence of the heuristics. Fuzzy set theory can represent descriptive relations, such as those between adjectives and nouns, hence the term descriptor for the relation defining a fuzzy set. In this case, the descriptors will contain the knowledge represented by the heuristics. Such a function should be an accurate description of the knowledge; but how rigorous must it be? Heuristics are developed based on knowledge of generalities and, as such, are widely applicable and inherently nonrigorous. More attention should, therefore, be given to developing accurate, rather than rigorous, descriptors.

Recall, that a descriptor defines a normalized set if there are elements in the universe that completely belong to that set. The design space consists of all possible separation sequences. The separation-task set consists of all possible separation tasks. Therefore, both the design space and the separation-task set are classical discrete sets. The heuristics describe characteristics of individual separation tasks. In this sense, heuristics can be thought of as fuzzy separation-task sets.

Heuristic: Eliminate Forbidden Separations. Based on the suggestion of Seader and Westerberg (1977), separations for which $\alpha \leq 1.05$ are forbidden. Therefore, only separations corresponding to $\alpha > 1.05$ will be considered. Equivalently, only λ cuts where $\alpha > 1.05$ will be taken.

Heuristic: Prefer Easy Separations. What defines an easy separation? Suppose that we refer to separations that require relatively few theoretical stages as easy. A descriptor can be developed based on consideration of the Fenske Equation (Henley and Seader, 1981), which can be written as Eq. 8:

$$N_{\min} = \frac{\log\left[\left(\frac{d_i}{d_j}\right)\left(\frac{b_j}{b_i}\right)\right]}{\log \alpha_{i,j}} \tag{8}$$

For the sake of example, we assume 98% recoveries of both keys for all separation tasks. For the sake of clarity, $\alpha_{i,j}$ will be replaced by α. Equation 8 can be rewritten as Eq. 9:

$$N_{\min}=\frac{2\log[(49)]}{\log\alpha} \tag{9}$$

Equation 9 decreases monotonically and asymptotically approaches zero as α tends to infinity. The rate of change of $N_{\min}$ with respect to α is given by Eq. 10:

$$\frac{dN_{\min}}{d\alpha}=-\frac{2\log[(49)]}{(\log\alpha)^2\alpha} \tag{10}$$

At large values of α, the rate of change in $N_{\min}$ with respect to α is small and separations are easy. Similarly, for small values of α the rate of change in $N_{\min}$ is large. Therefore, more information is contained about the ease of a separation in the region where the rate of change in $N_{\min}$ is significant. For our purposes the maximum rate of change in $N_{\min}$ occurs at $\alpha=1.05$. Suppose we say that separations corresponding to rates of change in $N_{\min}$ less than 1% of the maximum rate of change are easy, that is separations where $\alpha\geq1.5$ are easy. Therefore, the descriptor function should be defined over the interval $1.05\leq\alpha\leq1.5$. The largest value of $N_{\min}$ over the interval of interest is 160 at $\alpha=1.05$. The descriptor should increase as $\alpha\rightarrow1.5$ and go to zero as $\alpha\rightarrow1.05$. A descriptor is, therefore, obtained by dividing Eq. 9 by the maximum value of 160 and subtracting the result from unity as in Eq. 11:

$$\phi(\alpha)=\begin{cases}1-\dfrac{\log[(49)]}{80\log\alpha} & 1.05<\alpha\leq1.5\\ 0 & \alpha\leq1.05\end{cases} \tag{11}$$

This descriptor is plotted over the interval $1.05\leq\alpha\leq1.5$ in Figure 1. Notice the descriptor is not normalized. However, since there are separations that entirely belong to the set of easy separations, $\phi(\alpha)$ is not an accurate descriptor over the interval of interest. $\phi(\alpha)$ does provide insight to the behavior of the set relative to α.

Recall, from the definition of fuzzy complimentation, that

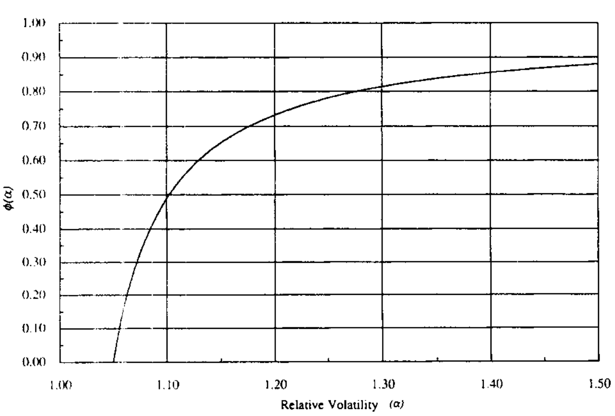

Figure 1. Heuristic descriptor, $\phi(\alpha)$, for the set of easy separations.

separations which correspond to $\alpha<1.1$ represent the higher degrees of membership in the set of "not-easy" separations, that is, difficult separations. Thus, an accurate descriptor will possess a crossover point at $\alpha\approx1.1$. A descriptor, based on a sigmoid, can be adjusted to achieve the desired characteristics. Such a function is presented in Eq. 12 and Figure 2.

$$\mu(\alpha)=\begin{cases}\left[1+e^{-\left(\frac{\alpha-1.1}{0.014}\right)}\right]^{-1} & 1.05<\alpha\leq1.5\\ 0 & \alpha\leq1.05\end{cases} \tag{12}$$

This descriptor is normalized and maintains the crossover point at $\alpha=1.1$. Note the crossover point corresponds to $N_{\min}\approx80$ so the interval $1.05\leq\alpha\leq1.1$, approximately, corresponds to $80\leq N_{\min}\leq160$. The descriptor $\mu(\alpha)$ qualitatively contains the same information as $\phi(\alpha)$. Since descriptors need not be uniquely defined, $\mu(\alpha)$ can be used to represent the set of easy separations.

Heuristic: Prefer Equimolar Separations. In this case, the term equimolar means that the mole flow rates of the distillate and bottom products are nearly equal. Clearly, the descriptor must be normalized and centered at the value that corresponds to a perfectly equimolar separation. Let the mole flow fraction, ρ, be defined as the bottoms to feed ratio that would result from the complete separation of the light and heavy keys. The cost of the separation task is related to the vapor rate in the column. Fractions corresponding to lower vapor rates, $\rho>0.5$, should be favored over those corresponding to higher vapor rates, $\rho<0.5$. The descriptor, $\varphi(\rho)$, for this heuristic is presented in Eq. 13, and Figure 3.

$$\varphi(\rho)=\begin{cases}e^{-\left(\frac{\rho-0.5}{0.01}\right)^2} & \rho<0.5\\ 1-30(\rho-0.5)^2 & \rho>0.5\end{cases} \tag{13}$$

The first heuristic requirement of $\alpha>1.05$ and the heuristic descriptors, $\mu(\alpha)$ and $\varphi(\rho)$, are combined in Eq. 14 to generate the total descriptor, $\Lambda(\rho,\alpha)$, that represents the set of preferred separations:

$$\Lambda(\rho,\alpha)=\begin{cases}\dfrac{\varphi(\rho)+\mu(\alpha)}{2} & 1.05<\alpha\leq1.5\\ 0 & \alpha\leq1.05\end{cases} \tag{14}$$

The heuristics represented by $\Lambda(\rho,\alpha)$ are weighted equally. For the purposes of this study, both are considered equally important for the development of a good design. The combination of these heuristic descriptors in this fashion has the desirable effect of resolving heuristic conflicts between $\mu(\alpha)$ and $\varphi(\rho)$. For example, a separation that has $\mu(\alpha)=0.7$ and $\varphi(\rho)=0.6$ ($\Lambda(\rho,\alpha)=0.65$) is favored over one for which $\mu(\alpha)=0.8$ and $\varphi(\rho)=0.3$ ($\Lambda(\rho,\alpha)=0.55$). Another form of conflict arises from the selection of the next separation task. Consider the set of next separation tasks as defined by taking progressively larger λ-cuts of $\Lambda(\rho,\alpha)$, say $\lambda\in\{0.95, 0.90, \ldots, 0.35\}$, until a potential separation is identified, that is, $\Lambda_\lambda(\rho,\alpha)\neq\Lambda_\varnothing(\rho,\alpha)$. The set described by $\Lambda_\lambda(\rho,\alpha)$ can contain more than one separation task. For example, say that $\lambda=0.75$ and that $\Lambda_\lambda(\rho,\alpha)$ contains two elements; $\Lambda(\rho,\alpha)=0.77$ and $\Lambda(\rho,\alpha)=0.79$. Are the al-

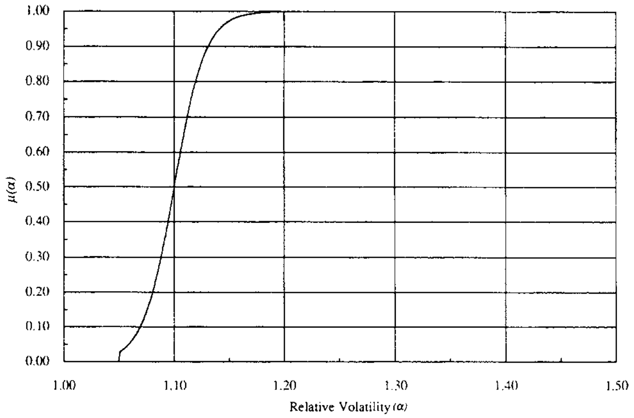

Figure 2. Heuristic descriptor, $\mu(\alpha)$, for the set of easy separations.

ternatives significantly different? In this case, fuzzy logic provides a fuzzy answer. Both separations should be evaluated by process simulation and the least expensive selected.

The descriptor, $\Lambda(\rho, \alpha)$, has been developed from analytic and qualitative arguments and contains the knowledge held in the three heuristics. Other heuristic descriptors can be developed in an analogous fashion. Finally, fuzzy descriptors can be developed which represent analytic approaches such as: marginal price (Modi and Westerberg, 1992), coefficient of ease of separation (Nadgir and Liu, 1983), or rule of thumb equation (Porter and Momoh, 1991).

Program Development

The distillation sequence synthesis system, DSEQSYS, develops sequences for the separation of a feed stream into its constituent components. The feed stream is specified as a saturated liquid at a given temperature and composition. Additionally, the light and heavy key recoveries are specified. The system consists of three separate components: a fuzzy heuristic synthesis program, a process simulator, and a batch control program. The fuzzy heuristic synthesis program is written in Microsoft FORTRAN 5.1. ASPEN PLUS™ is used to perform design simulations, equipment sizing, and process cost anal-

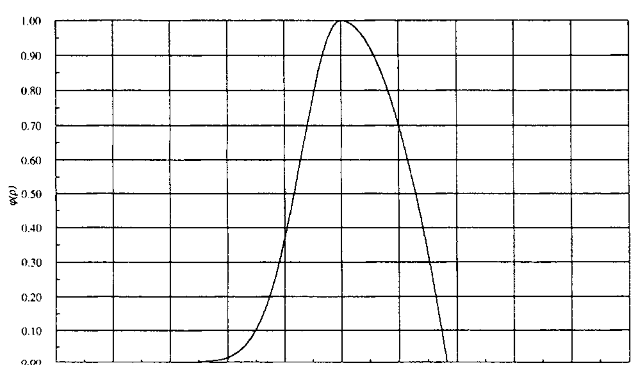

Figure 3. Heuristic descriptor, $\varphi(\rho)$, for the set of equal molar separations.

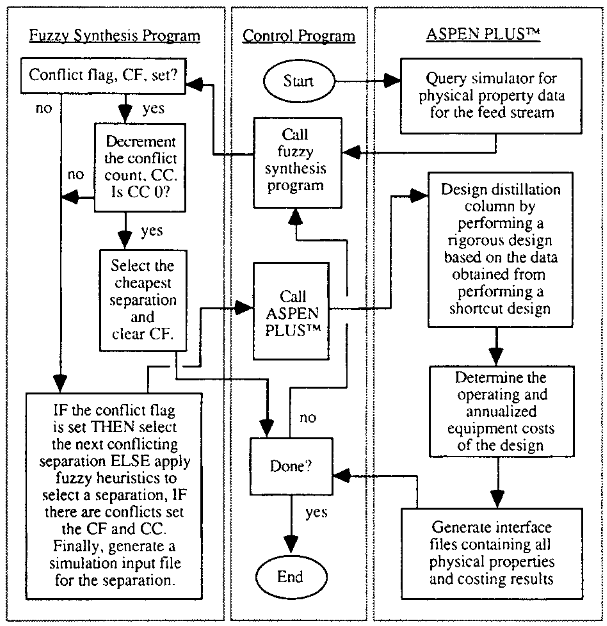

Figure 4. DSEQSYS flow diagram.

ysis. A MS-DOS batch program controls the execution of the synthesis program and the simulations. A flow diagram for DSEQSYS is given in Figure 4.

DSEQSYS obtains initial physical property information by performing a flash calculation on the feed stream. Resulting physical property values are then written to an interface file. The physical property data are read by DSEQSYS and used in applying the fuzzy heuristics. Therefore, separations including those that are forbidden are always based on current stream conditions. An input file is generated and submitted for simulation after a separation is selected. First, a shortcut design is performed to determine the number of theoretical stages and the feed stage location for the separation. This shortcut design also provides estimates for the reflux ratio, reboiler heat duty, and condenser heat duty. These values are used as a basis for rigorous distillation design. The desired key recoveries are achieved by simultaneously adjusting the reflux ratio and the reboiler duty during the rigorous design. The rigorous design results are then used to perform sizing and costing calculations. Finally, physical property data, for the distillate and bottom streams, are written to the interface file. The DSEQSYS continues performing syntheses and simulations until all separations have been performed or identified as forbidden.

The incorporation of a process simulator provides a convenient method of addressing nonideal and nonlinear behavior, as well as estimating equipment and operating cost. For instance, equations of state or activity coefficient models that are consistent with the chemical behavior of the mixtures under the design conditions are easily applied. Therefore, many of the simplifying assumptions typically used in heuristic based designs are not necessary. The physical properties of the distillate and product streams are based on rigorous heat and material balances. This information allows accurate results to be obtained from the heuristics at every stage of the design process and provides quantitative results. Detailed cost analyses are based on materials of construction, utility costs, and

Table 1. Cost and Sizing Data

Column Material	Carbon Steel
Tray Material	Carbon Steel
Tray Type	Sieve
Tray Efficiency	0.8
Steam Pressure	310 kPa
Steam Cost	\$3.60/1,000 kg
Brine T rise	15°C
Brine Cost	\$0.12/1,000 kg

Table 2. Problem 1 Data

Stream Temperature, 300 K		
	Component	Fraction
A	Propane	0.05
B	*i*-Butane	0.15
C	*n*-Butane	0.25
D	*i*-Pentane	0.20
E	*n*-Pentane	0.35

equipment performance. The cost analysis results provide a simple and efficient solution to heuristic conflicts.

Examples

Five example problems will be presented. For the sake of comparison with previous studies, three example problems have been taken directly from the literature (Heaven, 1969; Gomez and Seader, 1985; Wankat, 1988). The rigorous simulation and costing of all possible sequences for these three examples has been performed using ASPEN PLUS™. Two additional examples, that are modified literature examples, are also presented (Gomez and Seader, 1985; Cheng and Liu, 1988). These two problems demonstrate particular strengths of DSEQSYS. Sequence development time was approximately 10 min using a 66 MHz 486 personal computer.

Pure component physical property data were available for all chemical species in the ASPEN PLUS™ Pure Component Database. Nonideal vapor phase behavior was represented by the Redlich-Kwong equation of state. The representation of nonideal liquid behavior was accomplished using activity coefficients determined by the UNIFAC group contribution method. All separations were designed for 98% recoveries of the heavy and light keys at one atmosphere unless otherwise noted.

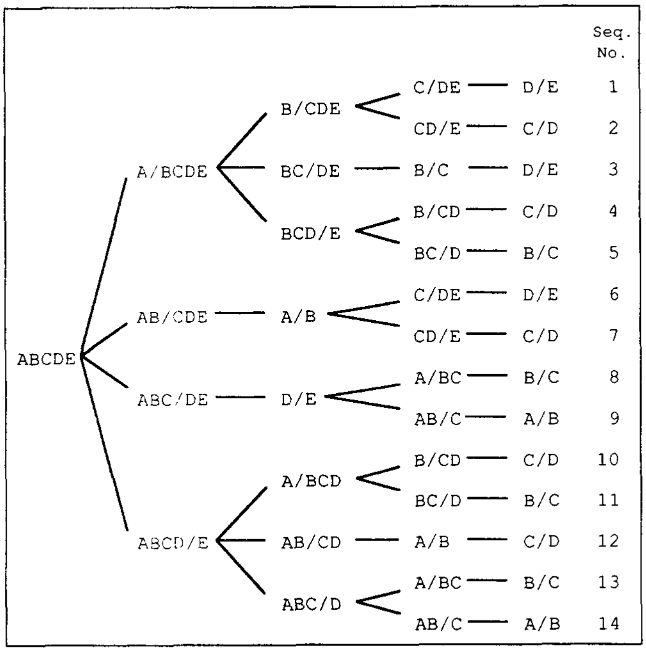

Figure 5. Sequence diagram for a five component separation.

Cost analysis data are presented in Table 1. Utility costs are based on data given by Peters and Timmerhaus (1990) for steam and cooling water. Equipment costs are annualized at a discounted-cash-flow rate of return of 15% over a 10 year period. An annualized cost is estimated using a capital charge factor (CCF) defined by Douglas (1988). The equipment costs include the entire column, condenser, and reboiler. Sizing of the condenser and reboiler is based on required duties and the utility conditions. The feed rate basis for each problem is 100 mol/s unless otherwise indicated.

Four of the problems involve five component separations. For a five component separation there are 14 possible separation sequences. For convenience each of these sequences is assigned an identification number, as shown in Figure 5. Subsequent cost analysis results are presented in terms of these identifiers.

Problem 1

An example reported by Heaven (1969) has been thoroughly studied in the literature. The problem specifications are given in Table 2. The brine inlet temperature was −15°C and the design pressure was 5 atm. DSEQSYS developed sequence 9 which is presented in Figure 6. This result is in agreement with Heaven (1969) and others (Nadgir and Liu, 1983; Douglas, 1985; Porter and Momoh, 1991). The annual cost of each of the 14 possible sequences is presented in Table 3.

The sequence developed by DSEQSYS is indicated by boldface type. Minimum costs are also indicated by boldface numbers. Note that the results from the synthesis system are not optimal. The optimal design corresponds to sequence 12. However, sequence 9 is optimal in equipment cost. Comparing sequence 9 to sequence 12 shows that there is only 0.35% difference in the annual cost. Further, there are 4 suboptimal designs which are within 1.3% (\$50,000) of the optimal design. Suboptimal sequences, such as these, have been reported by Douglas (1985) and Nadgir and Liu (1983).

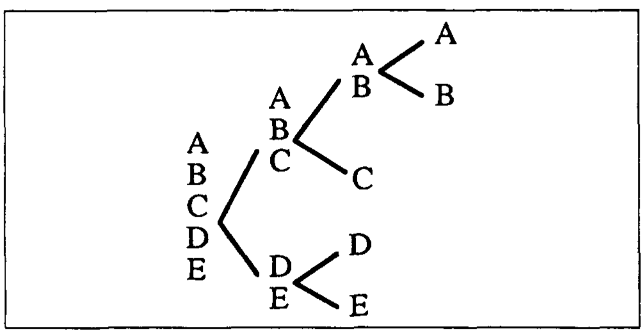

Figure 6. Separation sequence for problem 1.

Table 3. Detailed Cost Analysis for Problem 1

Seq. No.	Total Unit Cost	Annualized Equipment Cost	Annual Utility Cost Steam	Annual Utility Cost Brine	Total Annual Cost
1	$4,882,064	$1,713,604	$1,253,700	$1,129,100	$4,096,404
2	$5,025,545	$1,763,966	$1,210,900	$1,088,800	$4,063,666
3	$4,858,031	$1,705,169	$1,209,400	$1,087,400	$4,001,969
4	$4,990,153	$1,751,543	$1,190,800	$1,069,900	$4,012,243
5	$5,001,297	$1,755,455	$1,194,800	$1,073,700	$4,023,955
6	$4,754,892	$1,668,967	$1,188,800	$1,068,000	$3,925,767
7	$4,897,673	$1,719,083	$1,145,500	$1,027,200	$3,891,783
8	$4,792,596	$1,682,201	$1,184,100	$1,063,600	$3,929,901
9	**$4,744,011**	**$1,665,148**	$1,157,500	$1,038,600	$3,861,248
10	$4,771,223	$1,674,699	$1,159,400	$1,040,300	$3,874,399
11	$4,995,523	$1,753,428	$1,170,300	$1,050,600	$3,974,328
12	$4,877,503	$1,712,003	**$1,126,400**	**$1,009,300**	**$3,847,703**
13	$4,947,468	$1,736,561	$1,161,900	$1,042,700	$3,941,161
14	$4,899,026	$1,719,558	$1,135,400	$1,017,700	$3,872,658
Min.	$4,744,011	$1,665,148	$1,126,400	$1,009,300	$3,847,703

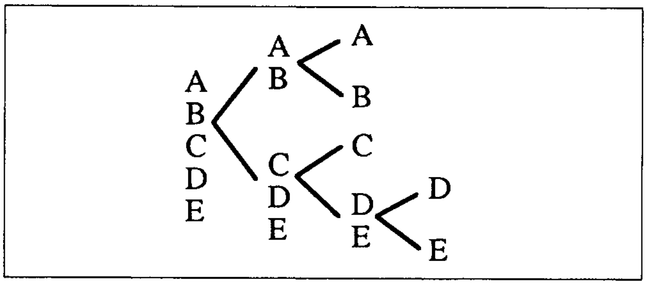

Figure 7. Separation sequence for problem 2.

Table 5. Detailed Cost Analysis for Problem 2

Seq. No.	Total Unit Cost	Annualized Equipment Cost	Annual Utility Cost Steam	Annual Utility Cost Brine	Total Annual Cost
1	**$2,105,032**	**$738,866**	$716,300	$538,500	$1,993,666
2	$2,280,998	$800,630	$776,500	$595,600	$2,172,730
3	$2,191,034	$769,053	$716,700	$538,900	$2,024,653
4	$2,405,138	$844,203	$817,000	$633,800	$2,295,003
5	$2,456,968	$862,395	$831,900	$647,900	$2,342,195
6	$2,112,900	$741,628	**$691,000**	**$514,500**	**$1,947,128**
7	$2,288,809	$803,372	$751,200	$571,600	$2,126,172
8	$2,276,300	$798,981	$754,200	$574,400	$2,127,581
9	$2,299,855	$807,249	$746,000	$566,600	$2,119,849
10	$2,840,417	$996,986	$813,600	$635,400	$2,445,986
11	$2,656,501	$932,432	$858,400	$677,500	$2,468,332
12	$2,631,074	$923,507	$809,600	$631,200	$2,364,307
13	$2,801,458	$983,312	$883,400	$701,100	$2,567,812
14	$2,825,071	$991,600	$875,200	$693,400	$2,560,200
Min.	$2,105,032	$738,866	$691,000	$514,500	$1,947,128

Problem 2

This example is based on a problem attributed to Gomez and Seader (1985). The problem is specified in Table 4. It was necessary to reduce the recovery of the heavy key to 95% for meaningful cost analysis results. DSEQSYS developed sequence 6, which is presented in Figure 7. These results are consistent with those reported by Gomez and Seader (1985). They developed sequence 6 by application of the thermodynamic search (TS) algorithm. The cost of each of the possible 14 sequences is presented in Table 5. Notice, in this case DSEQSYS developed the optimal sequence. However, sequence 1, is optimal in equipment cost. Further, sequence 1 is also near optimal (within $50,000).

Problem 3

An example attributed to Wankat (1988) is presented in Table 6. This example demonstrates nonideal behavior. The UNIFAC group contribution method was used to estimate liquid-phase activity coefficients. The Redlich-Kwong equation of state was used to estimate vapor-phase behavior. Sequence 6 was developed by DSEQSYS and is presented in Figure 8. These results are consistent with those reported by Wankat (1988). A detail sequence cost analysis for this problem is presented in Table 7. The sequence identified by DSEQSYS is optimal. However, sequence 1 is optimal in operating cost. Further, sequence 1 is the only near optimal (within $50,000) solution.

Problem 4

This problemm is a modification of problem 2. The problem is specified in Table 8. The only difference between problem 2 and this problem is that the mole fractions of *n*-Heptane and *n*-Octane have been changed. This change results in two separation tasks being selected for the initial separation. This sort of conflict cannot be dealt with, in a general manner, by expert systems or fuzzy logic alone. However, DSEQSYS provides a simple solution to the problem. All selected separation tasks are simulated and the task resulting in the least expensive separation is selected. In this case, the two separation tasks selected for the initial separation are AB/CDE and ABC/DE. Both separations are simulated resulting in costs of $307,080 for AB/CDE and $504,959 for ABC/DE. Thus, separation AB/CDE is selected. The sequence 6 developed by DSEQSYS is shown in Figure 9.

Table 4. Problem 2 Data

	Temperature, 300 K	
	Component	Fraction
A	*n*-Pentane	0.15
B	*n*-Hexane	0.20
C	*n*-Heptane	0.30
D	*n*-Octane	0.20
E	*n*-Decane	0.15

Table 6. Data for Problem 3

	Temperature, 300°C	
	Component	Fraction
A	Ethanol	0.25
B	*i*-Propanol	0.15
C	*n*-Propanol	0.35
D	*i*-Butanol	0.10
E	*n*-Butanol	0.15

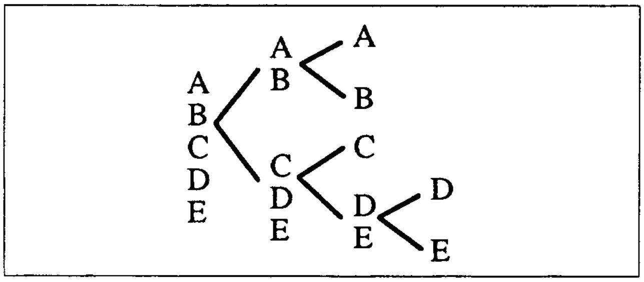

Figure 8. Separation sequence for problem 3.

Table 7. Detailed Cost Analysis for Problem 3

Seq. No.	Total Unit Cost	Annualized Equipment Cost	Annual Utility Cost Steam	Annual Utility Cost Brine	Total Annual Cost
1	$5,384,873	$1,890,090	**$2,052,500**	**$1,857,100**	$5,799,690
2	$5,510,606	$1,934,222	$2,178,100	$1,976,100	$6,088,422
3	$5,392,803	$1,892,874	$2,094,000	$1,896,500	$5,883,374
4	$5,590,676	$1,962,327	$2,204,200	$2,000,800	$6,167,327
5	$5,559,569	$1,951,409	$2,272,400	$2,065,400	$6,289,209
6	**$5,135,023**	**$1,802,393**	$2,069,800	$1,873,500	**$5,745,693**
7	$5,260,756	$1,846,525	$2,195,400	$1,992,500	$6,034,425
8	$6,003,287	$2,107,153	$2,186,200	$1,983,700	$6,277,053
9	$5,793,760	$2,033,610	$2,244,200	$2,038,700	$6,316,510
10	$5,538,614	$1,944,053	$2,252,400	$2,046,500	$6,242,953
11	$5,675,964	$1,992,263	$2,345,800	$2,134,900	$6,472,963
12	$5,505,331	$1,932,371	$2,329,800	$2,119,800	$6,381,971
13	$6,292,242	$2,208,577	$2,450,000	$2,233,500	$6,892,077
14	$6,082,550	$2,134,975	$2,508,000	$2,288,500	$6,931,475
Min.	$5,135,023	$1,802,393	$2,052,500	$1,857,100	$5,745,693

Problem 5

This example is based on a problem presented by Cheng and Liu (1988). The problem is specified in Table 9. The sequence developed by the synthesis system is shown in Figure 10. Forbidden separations ($\alpha \leq 1.05$) are indicated by boldface in Figure 10. This example demonstrates the ability of the design system to handle practical problems that consist of many components and contain forbidden separations.

Conclusion

DSEQSYS, a system exploring automated synthesis of distillation sequences based on fuzzy heuristics and process simulation has been presented. It has been demonstrated that the development of fuzzy heuristics is simple, requiring little formal knowledge of fuzzy set theory and that fuzzy heuristics are easily implemented in standard programming languages such as FORTRAN. A simple method for heuristic conflict resolution has also been shown.

The performance of DSEQSYS was demonstrated by the analysis of several example problems. In the cases where the example problems were selected from the literature (problems 1, 2 and 3), DSEQSYS reproduced the reported results. Example problem 3 demonstrates the use of process simulation to address the problems of nonideal and nonlinear behavior. With very little additional effort DSEQSYS was able to accommodate the highly nonideal liquid-phase behavior and provide a solution. A method for heuristic conflict resolution was demonstrated in problem 4. In this case, fuzzy heuristics alone proved inadequate to resolve the problem. However, using process simulation DSEQSYS was able to provide a simple quantitative solution. Problem 5 demonstrates the extension of DSEQSYS to larger problems that involve forbidden splits.

Table 8. Problem 4 Data

Temperature, 300 K		
	Component	Fraction
A	*n*-Pentane	0.15
B	*n*-Hexane	0.20
C	*n*-Heptane	0.25
D	*n*-Octane	0.25
E	*n*-Decane	0.15

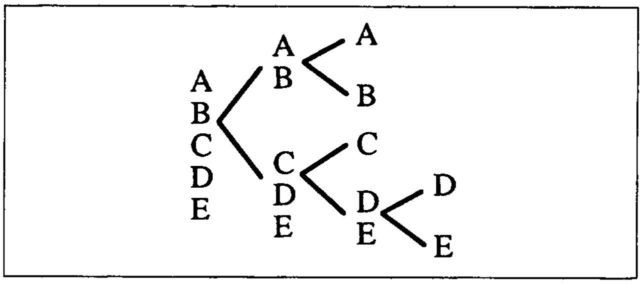

Figure 9. Separation sequence for problem 4.

Table 9. Problem 5 Data

Temperature 300°C		
	Component	Flow Rate
A	22DMP	32.51
B	*i*-Pentane	59.96
C	*n*-Pentane	62.69
D	22DMB	6.63
E	23DMB	10.81
F	2MEP	62.72
G	*n*-Hexane	39.61
H	Benzene	80.33

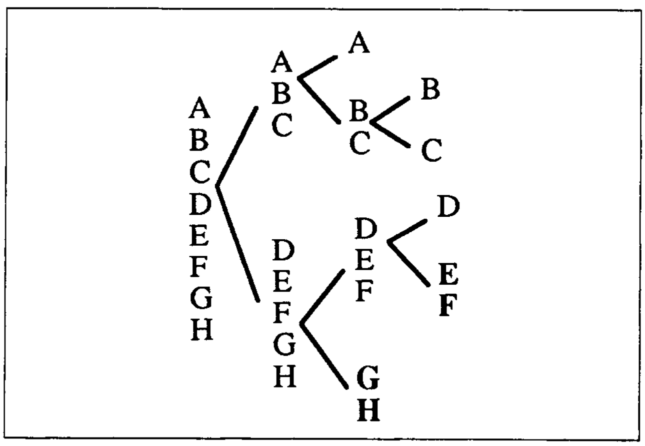

Figure 10. Separation sequence for problem 5.

Accommodating nonideal behavior is necessary for developing practical designs; therefore, DSEQSYS provides a significant advantage over other heuristic approaches. Also, the ability to identify and resolve heuristic conflicts makes DSEQSYS superior to expert systems. Additionally, DSEQSYS provides advantages over the mathematical programming approach. First, since DSEQSYS is heuristic based, it can generate process flowsheets without relying on a prespecified superstructure. Secondly, program modification is not required for varying design constraints and process variables. Changes to the design constraints and process variables are conveniently accomplished by simply editing the appropriate simulation input files.

Results indicate that this hybrid approach provides a more powerful and versatile design environment than that provided by heuristics, mathematical programming, or simulation alone.

Notation

A, B, C, . . . = component identifiers sorted based on k values (A largest)
A = arbitrary fuzzy set
$\bar{A}$ = complement of arbitrary fuzzy set A
A_λ = λ cut of arbitrary fuzzy set A
b_i = light key flow rate in bottom stream
b_j = heavy key flow rate in bottom stream
d_i = light key flow rate in distillate stream
d_j = heavy key flow rate in distillate stream
i = light key
j = heavy key
$\max(a, b, \ldots)$ = maximum value in list $(a, b, \ldots)$
$\min(a, b, \ldots)$ = minimum value in list $(a, b, \ldots)$
n = number of separation tasks
$N_{\min}$ = minimum number of stages required for separation
S_n = number of possible sequences for n separation tasks
supp A = support of fuzzy set A
U = universe of fuzzy sets
x = arbitrary element of fuzzy set

Mathematical conventions

$\in$ = element of
$\exists$ = there exists
$\forall$ = for all
$\varnothing$ = null or empty set

Greek letters

$\alpha_{i,j}$ = relative volatility of i to j
α = same as $\alpha_{i,j}$
λ = positive nonzero real value less than or equal to 1
$\Lambda(\rho, \alpha)$ = fuzzy heuristic descriptor
$\mu(\alpha)$ = fuzzy heuristic descriptor
$\mu_A(x)$ = arbitrary fuzzy descriptor for set A
$\mu_{\bar{A}}(x)$ = arbitrary fuzzy descriptor for the complement of set A
$\mu_\varnothing(x)$ = null or empty fuzzy set
$\mu_{A\cup B}(x)$ = arbitrary fuzzy descriptor for set A union B
$\mu_{A\cap B}(x)$ = arbitrary fuzzy descriptor for set A intersect B
ρ = bottoms to feed ratio
$\phi(\alpha)$ = fuzzy heuristic descriptor
$\varphi(\rho)$ = fuzzy heuristic descriptor

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