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A combined method for the design and optimization of intensified distillation systems

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ABSTRACT

The sequential design method (SDM) is a recently introduced distillation column design method based on the correspondence between the simple column and the alternative sequences design parameters. It can be defined as a method that combines the alternatives generation step with the design procedure. The Multi-Objective Differential Evolution (MODE) algorithm instead, is based on the minimization or maximization of a defined objective function; it is a strong method that allows the evaluation of a large number of alternatives.

The SDM is characterized by a poor control of the error propagation among the sequences, the MODE algorithm by a high computational time. It was obtained that a proper combination of the methods allows the compensation of the drawbacks of the stand-alone procedures. For the case study considered, when the MODE algorithm is initialized with the SDM, a 39% reduction of the computational time was observed. If the combination between the methods is realised at the beginning of the design procedure, the reduction of the computational time was of about 28%. The time reduction was due to a narrower initialization of the MODE algorithm with the parameters obtained applying the SDM. Moreover, when some overestimated design values where used to initialize the MODE algorithm, it is still possible to identify a configuration very close to the optimum.

1. Introduction

The separation of a multicomponent mixture into different commercial products passes through the identification of the optimal separation sequence. The procedure to obtain the final design includes five main steps:

1. definition of the separation method
2. generation of the alternatives
3. design of the alternatives
4. screening of the alternatives by means of an objective function
5. selection of the best alternative.

Regarding the first point, if applicable, distillation remains the most widespread separation methods at industrial scale [1]. The second step represents one of the most discussed open issue in the chemical engineering research community moving from synthesis of heat integrated sequences [2], separation of azeotropic mixtures [3], sharp [4] and nonsharp separations [5] or configurations with a reduced number of columns [6].

For many years the prediction of a complete searching space that includes all, or most of the possible distillation sequences, has been considered independently from the design method used for the economic evaluation of each single sequence. From one point of view this approach can be considered reasonable. The available distillation's design methods are nowadays mature and reliable [7–11]. Moreover simulation software packages like Aspen Plus speeded up even more the design procedure. It is a well-known procedure that, when a multicomponent mixture is separated by distillation, the simple column (SC) sequences are the first alternatives considered. These sequences are usually preferred

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Nomenclature

B	($kmol\,h^{-1}$) bottom flowrate
CC	($\$\,y^{-1}$) capital cost
Ci	(i = 1,4) column number
Cr	crossover probability
D	($kmol\,h^{-1}$) distillate flowrate
F	mutation factor
G	number of generations
LW	($kJ\,h^{-1}$) lost work
N	number of stages
N_F	feed stage
N_p	size of population
N_S	side stream stage
P_c	(bar) column pressure
Q_c	(kW) condenser duty
Q_r	(kW) reboiler duty
RR	reflux ratio
S	($kmol\,h^{-1}$) side stream flowrate
TAC	($\$\,yr^{-1}$) total annual cost
W_{min}	($kJ\,h^{-1}$) minimum work of separation
x_F	feed molar fraction
x_m	vector of product purity restrictions defined by the designer for m components
x_P	product molar fraction
x_{var}	decision variable for optimization
y_m	vector of product purities obtained through rigorous simulation for m components
Φ	(m) column diameter
η	thermodynamic efficiency

because of the easiness of the design and control and their diffusion in the industrial practice. For all these reasons, simple column sequences are the term of comparison for all the alternatives predicted and considered [12].

This last point expresses very clearly that, at the beginning of the alternatives screening phase, the designer has already designed and identified the best, or the sub set of best, simple column sequences.

In previous studies [13–15] the main research work was focused on developing a systematic method that, starting from the simple column sequences, allows the designer to predict a wide set of alternatives including; thermally coupled, thermodynamic equivalent, intensified sequences and even divided wall columns. The whole searching space of distillation sequences can be decomposed in different subspaces each with specific features. The subspace of simple column sequences includes only simple columns formed by a single feed, a distillate and a bottom product. The subspace of thermally coupled sequences contains configurations with one or more bidirectional vapor–liquid stream between two consecutive columns, the subspace of the thermodynamically equivalent sequences is obtained recombining the column sections associated to a thermal coupling, the subspace of the intensified sequences is generated by substitution of a single column section (named transport section) by means of a side stream, finally the divided wall columns are considered as the ultimate possibility to obtain more than two products from a single distillation column.

The motivation to keep this strict connection between simple column sequences and the subspaces of alternatives, derived from the evidence that the sequences obtained from the best simple column sequence are still the best among all the alternatives.

Applying this concept to the identification of the best distillation sequence, it is possible to define first a sub set of best simple column sequences, then, considering only the alternatives derived from them, it is possible to limit the design calculations to a reduced set of alternatives making the screening phase faster. This modus operandi relates the alternatives generation method to the possibility of calculation reduction, but the design method used still remains an independent issue. Following this headway the goal is to define a procedure that connects each simple column sequence's design with the design of the alternatives included in the searching space.

For this reason, a design method called Sequential Design Method (SDM) was introduced as a complementary tool to the systematic prediction of the distillation sequences alternatives [16]. The method is based on the correspondence among the column sections functionality of the simple column sequences and the corresponding alternatives. Despite its simplicity, the SDM was proved to be a reliable design method even compared to methods based on strong mathematical background like the Multi-Objective Differential Evolution (MODE) optimization algorithm, able to minimize different objective functions screening large amounts of alternatives by means of the Pareto-optimal front generation technique.

The aim of the present work is to explore the possibility to integrate the SDM and the MODE algorithm. Differently to our previous work [16] where the SDM was introduced, the novelty of the present study is represented by a deep analysis on how is possible to overcome the drawbacks of the single design methodologies in order to obtain a fast and reliable design procedure.

A distillation sequence for a five-component mixture is considered as an example to prove the potential of the methodology.

2. Problem description

It is required to design the intensified distillation sequence reported in Fig. 1. For a five-component separation, the simple columns sequences are composed by four columns, since the sequence considered employs only three columns, is expected to be potentially more convenient. The sequence reported in Fig. 1 was identified as a Modified Simple Column (MSC) sequence because each product is obtained as a distillate or as a residue [15]. In the case of four-component mixtures it was proved that for some composition cases, the MSCs can realize a lower total annual cost compared to the simple column alternatives [14]. The CD side stream, below the column feed, is considered in the vapor phase according to the heuristic rules defined by Kim and Wankat [17] and confirmed by Errico et al. [13].

A saturated liquid feed of 100 kmol/h composed by n-paraffins at the pressure of 2 bar is considered. The feed composition and the product purity specifications are reported in Table 1.

All the sequences examined in the present work were designed by means of the software Aspen Plus. The NRTL method was used to

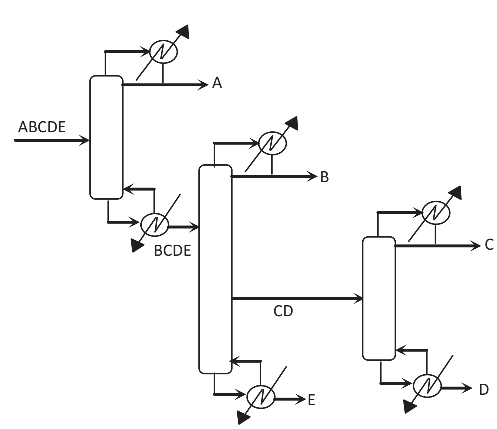

Fig. 1. Intensified sequence for a five component separation.

Table 1
Feed composition and required product purity.

Component	x_F	x_P
A: C_5H_{12}	0.35	0.999
B: C_6H_6	0.1	0.989
C: C_7H_{16}	0.1	0.990
D: C_8H_{18}	0.4	0.988
E: $C_{10}H_{22}$	0.05	0.979

estimate the liquid phase activity coefficients and the vapor phase was considered as ideal. The rigorous stage-to-stage equilibrium model for distillation columns RadFrac was chosen, together with total condensers and kettle reboilers. Considering that the components do not form any azeotrope and there are no recycle streams in the configuration, the default convergence settings were used. The Aspen Economic Analyzer was employed for the capital cost evaluation and an investment time of 10 years was considered. All the calculations were performed with an Intel Core i5, 2.67 GHz, 10 GB ram in Windows 7 environment (Ultimate edition 64 bit).

3. The sequential design method and the multi-objective differential evolution algorithm approach

The sequential design method relates the alternative sequence considered to the correspondent simple column sequence from which is generated. Once this correspondence is defined it is possible to transpose the design parameters between the analogous columns sections. A column section is defined as a set of stacked trays or packing where vapor–liquid equilibrium takes place and any other external mass or heat transfer does not take place. Analogous sections between two different distillation sequences are considered as sections that performed the same separation task. Focusing on the sequence reported in Fig. 1, the complete synthesis method is not relevant for the scope of the present work, however in Fig. 2 the derivation steps necessary to move from the simple column sequence to the MSC sequence, are reported. The complete generation procedure was developed by Rong and Errico [15] and here briefly recalled.

Table 2
Design parameters, energy consumption and capital costs of the SC of Fig. 2(a).

	C1	C2	C3	C4
N	42	47	29	36
N_F	31	29	17	21
P_C (bar)	1.6	1.0	1.0	1.0
D (kmol h^{-1})	35.00	10.10	50.20	9.90
B (kmol h^{-1})	65.00	54.90	4.70	40.30
RR	0.920	11.900	0.206	7.100
Φ (m)	0.73	1.07	0.81	0.90
ΣQ_c (kW)	−2878.48			
ΣQ_r (kW)	2965.11			
CC ($ yr^{-1})	257280			
TAC ($ yr^{-1})	1664038			
η	16.68			

From the simple column sequence of Fig. 2(a) it is possible to generate the thermally coupled (TC) sequence of Fig. 2(b), then recombining the column section 6 associated to the thermal coupling, the thermodynamically equivalent sequence (TES) of Fig. 2(c) is obtained. Finally substituting the transport section 5, the required sequence is reported in Fig. 2(d). It is evident that the SC sequences of Fig. 2(a) and the MSC in Fig. 2(d) are deeply connected and the SDM uses this correspondence to relate the design of the SC to the MSC. The first step to proceed with the SDM, is the design of the reference simple column sequence of Fig. 2(a). Using the simulation package Aspen Plus, the sequence was first simulated using the Underwood-Gilliland-Winn method to get the initial parameters (number of stages, feed location and reflux ratio), and then the final design was obtained using the rigorous model RadFrac. Taking into consideration the availability of cooling water in the condensers having inlet and outlet temperatures of 20 °C and 40 °C, respectively, the pressure of each column was optimized. The results obtained are summarized in Table 2.

Based on the correspondence between the column section functionality, the design parameters of the simple column sequence

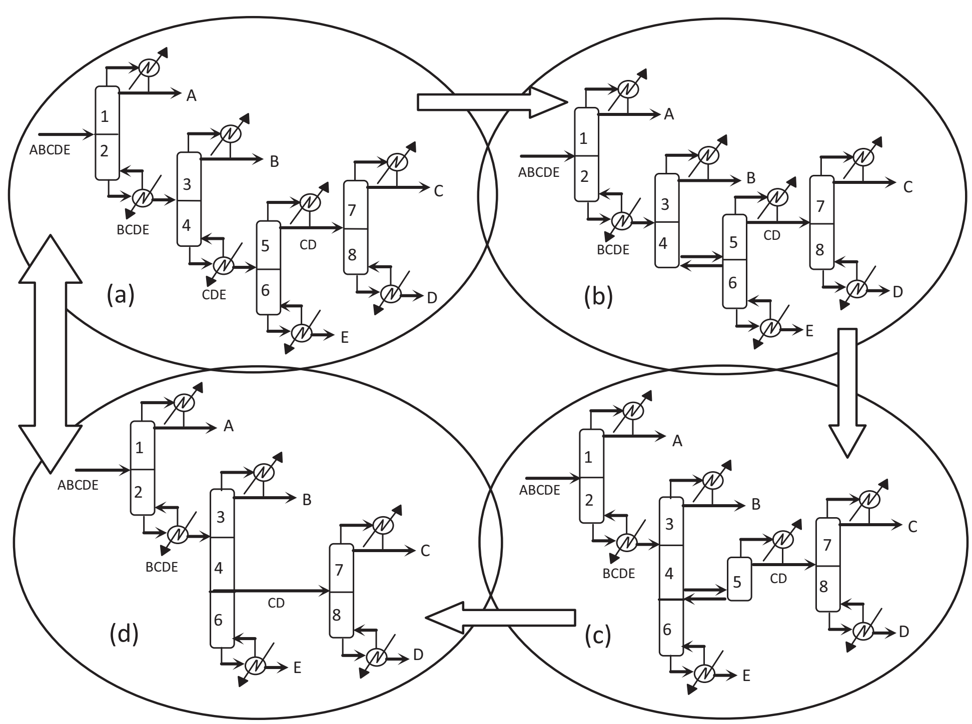

Fig. 2. Systematic procedure for the MSC sequence generation: (a) SC sequence, (b) TC sequence, (c) corresponding TES, (d) MSC sequence.

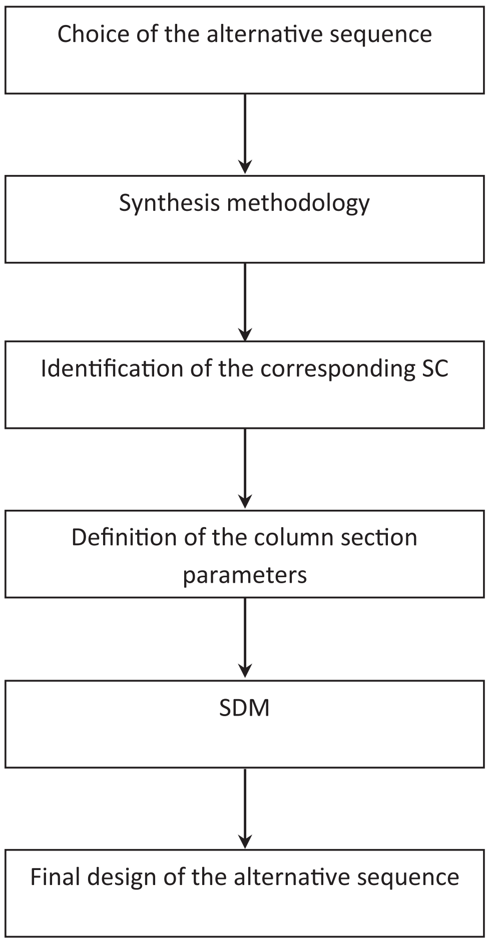

Fig. 3. SDM procedure.

were used to define those of the MSC configuration of Fig. 2(d). The whole procedure has been summarized in the flowchart of Fig. 3 where starting from the definition of the configurations to be designed, the corresponding SC sequence is identified following the synthesis methodology that includes the introduction of thermal couplings and the column section recombination. Once this connection is clearly identified is possible to identify the column section design parameters. As reported in the flowchart, using the SDM the design parameters of the SC sequence are transposed to the configuration initially selected in order to obtain the final design.

Table 3
SDM design parameters, energy consumption and capital costs of the MSC of Fig. 2(d).

	C1	C2	C3
N	42	56	36
N_F	31	30	15
P_C (bar)	1.6	1.0	1.0
N_s	–	47	–
D (kmol h^{-1})	35.00	10.10	9.90
B (kmol h^{-1})	65.00	4.70	40.30
S (kmol h^{-1})	–	50.20	–
RR	0.92	12.20	10.65
Φ (m)	0.73	1.34	1.05
ΣQ_c (kW)		−2630.44	
ΣQ_r (kW)		2717.01	
CC ($ yr^{-1})		233690	
TAC ($ yr^{-1})		1603316	
η		12.65	

Table 3 shown the results obtained. A mean time of six hours was necessary to get the final design. This time depends on the ability of the designer utilizing the simulation software.

It is possible to notice that, compare the SC, the MSC realized 9% reduction of the total condenser and reboiler duty and a 9% saving in the capital costs.

The MODE algorithm uses differential evolution (DE) as stochastic method for global optimization. DE is a population based direct search method especially recommended for nonlinear and non-differentiable continuous functions. It mimics biological evolution by performing generation (mutation and crossover), evaluation and selection as in genetic algorithm (GA). Compared to GA, the main advantages of DE are its capability to escape from the local optima and the faster convergence to the global optimum [18].

The DE inside the MODE algorithm has three main parameters: the size of population (N_p), the mutation factor (F) and the crossover probability (Cr) besides initialization of the population, selection of three random vectors in the mutation operation, and the convergence criteria. In general terms, a higher N_p increases the probability to identify the global optimum but slows down the convergence. Values between 5 and 20 times the number of decision variables optimized are recommended. Similarly, increasing F, increases the possibility to find the global optimum, penalizing the computational time. Values between 0 and 2 are suggested. DE is not very sensitive to Cr and usually values between 0 and 1 are defined. The tuning procedure of these parameters is out of the scope of the present work, and the initial values suggested by Rangaiah [19] were used. These values were estimated trying the DE in different challenged benchmark problems as presented by Price et al. [20].

The MODE convergence criterion is the number of generations (G). This criterion was fixed according to previously experience in other separation systems with similar, in nature and number, decision variables.

The objective functions used in the MODE to select the final design are the total annual cost (TAC) to be minimized and the thermodynamic efficiency (η) to be maximized.

The TAC was evaluated following the Guthrie's method [21]:

$$\min(\mathrm{TAC}) = \sum\left[\left(\frac{\text{Capital Cost}}{\text{Time of Investment}}\right) + (\text{Cost of Utilities})\right] \quad (1)$$

The thermodynamic efficiency was implemented according to the methodology reported by Seader et al. [22]:

$$\max(\eta) = -\frac{W_{\min}}{(-\mathrm{LW} - W_{\min})} \quad (2)$$

Once the objective functions and the decision variables are defined, the optimization problem for the MSC is given below:

$$\min(\mathrm{TAC}),\ \max(\eta)$$
$$= f(N_1, N_{F1}, RR_1, N_2, N_{F2}, N_{S2}, RR_2, N_3, N_{F3}, RR_3) \quad (3)$$

where the number indicates the column in the sequence (from left to right), subject to:

$$y_m \geq x_m \quad (4)$$

$$\mathrm{Limit}_{\mathrm{lower},\,var} \geq x_{var} \geq \mathrm{Limit}_{\mathrm{upper},\,var} \quad (5)$$

The thermodynamic efficiency was introduced to take into account the efficient energy usage and to screen among configurations with a similar annual cost.

When the design of the configuration of Fig. 2(d) is approached using the MODE algorithm, the designer has no indications about the column's parameters initialization. For this reason the arbitrary upper limit of 100 stages was considered for each column. The feed location was left free to vary along the column and the CD side stream of the second column was imposed to be below the feed

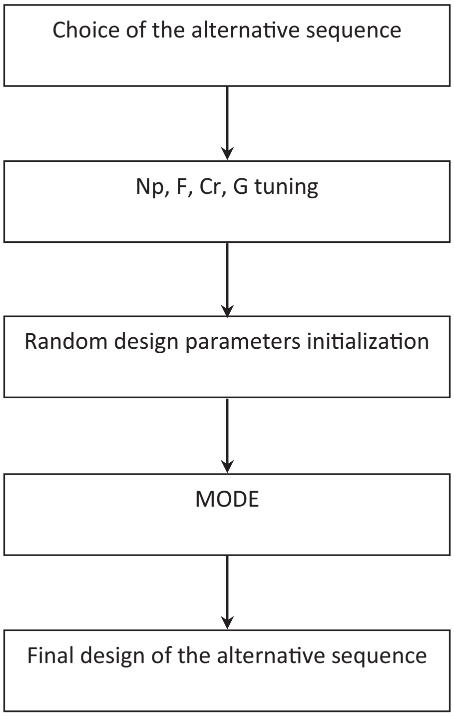

Fig. 4. MODE design procedure.

location and in vapor phase. The reflux ratio was varied in the range 0.1–20. The procedure described is summarized in the flowchart of Fig. 4. In this case after the choice of the sequence to be designed it is necessary to tuning the population size, the mutation factor, the crossover probability and the number of generation related to the mathematical method. Then, a first trial set of design parameters is necessary to initialize the MODE algorithm in order to get the final design.

The final design obtained is reported in Table 4.

Should be pointed out that in the MODE algorithm the capital costs were evaluated following a modular approach using the single unit capacity (e.g. column volume, exchanger area, etc.) to evaluate the base cost. In order to have a fair comparison with the SDM's results, the capital costs of the configuration selected were evaluated again with the Aspen Economic Evaluator.

The final solution was obtained after 89 h and 30 min. When the population size was 200, the number of individuals evaluated was 18404. The Pareto-optimal solutions for different generations are reported in Fig. 5. It is possible to notice that from generation 180 to generation 200 the difference is not meaningful, and the

Table 4
MODE design parameters, energy consumption and capital costs of the MSC of Fig. 2(d).

	C1	C2	C3
N	68	58	41
N_F	51	33	14
P_C (bar)	1.6	1.0	1.0
N_s	–	46	–
D (kmol h^{-1})	35.00	10.10	9.90
B (kmol h^{-1})	65.00	4.70	40.30
S (kmol h^{-1})	–	50.20	–
RR	0.85	12.11	10.65
Φ (m)	0.72	1.33	1.05
ΣQ_c (kW)		−2603.44	
ΣQ_r (kW)		2690.11	
CC ($ yr^{-1})		368330	
TAC ($ yr^{-1})		1723330	
η		12.81	

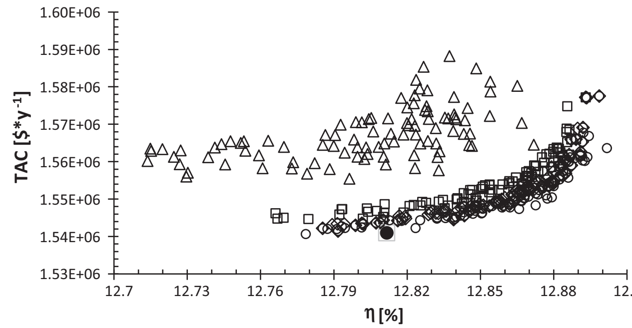

Fig. 5. Pareto-optimal solutions for different generations. △: G = 100, □: G = 150, ◇: G = 180, ○: G = 200, ●: selected design.

designs with the lowest TAC value are in the range of a reasonable thermodynamic efficiency.

Comparing the solutions obtained by the different methods reported in Tables 3 and 4, it is evident a general agreement in the final design. The difference in the total condenser and reboiler duty is about 2% and can be considered irrelevant. Only the capital costs for the solution obtained with the SDM are 37% less of the corresponding value obtained by the MODE algorithm.

Regarding the objective functions, it can be observed that because the energy consumption is slightly lower, the thermodynamic efficiency is barely higher for the sequence obtained by MODE algorithm. However, the capital cost had an important negative impact in the calculation of TAC, resulting in a 7.5% increasing with respect to the MSC estimated by the SDM.

4. SDM and MODE algorithm integration

Once the reference simple column sequence is identified, the sequential design method is certainly fast and easy to apply. On the other hand the main drawback is the propagation of errors from the simple column design to the alternative considered. In other words, if the designer makes an error in the definition of a parameter of the simple column sequence, this error is directly transferred to the alternative sequence design with poor possibilities of its detection.

The MODE algorithm, among the benefits, has a high probability to identify the optimal solution.

However, using the MODE, the designer has not any indication about the parameters initialization. For this reason it is necessary to explore a wide variation of the parameters even if the corresponding computational time could results excessive.

The aim of combining the two design approaches is justified by the possibility in the mutual reduction of the drawbacks associated to the methods when they are utilized independently.

It is important to notice that the integrations between the methods is allowed every time is possible to relate the distillation sequence considered to the correspondent simple column sequence. This relationship was already defined for a broad class of alternatives including extractive distillation sequences [23], heat integrated configurations [24], divided wall columns [25] and Petlyuk configurations [26].

4.1. MODE algorithm initialized by the SDM

In this case, the design parameters obtained applying the SDM are used to initialize the MODE algorithm. The correspondent solution is reported in Table 5. The optimization problem for this MSC sequence is the same already described in section 3, with the difference that the initialization was changed taking into account the SDM parameters.

Table 5
Design parameters, energy consumption and capital costs of the MSC of Fig. 2(d) obtained by the MODE algorithm initialized with the SDM.

	C1	C2	C3
N	50	68	44
N_F	37	31	16
P_C (bar)	1.6	1.0	1.0
N_s	–	51	–
D (kmol h^{-1})	35.00	10.10	9.90
B (kmol h^{-1})	65.00	4.70	40.30
S (kmol h^{-1})	–	50.20	–
RR	0.86	12.07	10.27
Φ (m)	0.72	1.33	1.04
ΣQ_c (kW)		−2573.70	
ΣQ_r (kW)		2660.35	
CC ($ yr^{-1})		286800	
TAC ($ yr^{-1})		1627618	
η		12.92	

Table 6
Design parameters, energy consumption and capital costs of the MSC of Fig. 2(d) obtained by the MODE algorithm initialized with overestimated SDM values.

	C1	C2	C3
N	50	62	44
N_F	36	32	16
P_C (bar)	1.6	1.0	1.0
N_s	–	51	–
D (kmol h^{-1})	35.00	10.10	9.90
B (kmol h^{-1})	65.00	4.70	40.30
S (kmol h^{-1})	–	50.20	–
RR	0.90	12.11	10.26
Φ (m)	0.73	1.33	1.04
ΣQ_c (kW)		−2584.98	
ΣQ_r (kW)		2671.68	
CC ($ yr^{-1})		284020	
TAC ($ yr^{-1})		1631540	
η		12.87	

Analyzing the results obtained for the SDM (Table 3), for the MODE algorithm (Table 4) and for their combination (Table 5), it is possible to notice that the design obtained combining the SDM with the MODE algorithm has a less energy consumption compared to the stand-alone design methods.

Utilizing the MSC design parameters obtained from SDM as starting point for the MODE algorithm, a general improvement in the objective functions was observed. For instance, the thermodynamic efficiency is slightly increased compare to the design obtained with the SDM or the stand-alone MODE algorithm. One of the main differences observed in the final design obtained applying the SDM or the MODE algorithm is related to the capital costs. When the methods are combined the correspondent capital cost is 22% less than the value obtained by the MODE algorithm alone. Consequently the TAC is only 1.5% higher than the MSC configuration obtained via SDM.

The computational time necessary to obtain the final design was 54 h and 40 min, which means a reduction of 39% compared to the stand-alone MODE algorithm with a broad initialization.

4.2. How to avoid the error propagation in the SDM

In this section the influence of design errors in the initialization of the MODE algorithm has been considered.

According to Fig. 2(a) and (d) the first column of the SC sequence is exactly the same in the MSC. Applying the SDM, the designer simply transposes the correspondent design values from the SC to the new sequence. In this case the designer has small chances to identify possible errors. Since the reflux ratio is directly related to the distillation column energy consumption, its estimation is critical for the overall economy of the separation. The reflux ratio of the SC sequence of Fig. 2(a) was changed from 0.92 to 1.1.

Then, using this value to initialize the MODE algorithm, the results reported in Table 6 have been obtained. The final solution was identified after 61 h and 30 min that is a value comparable with the previous case. It is also possible to notice that, regarding the objective function values, the configuration obtained is very close to the design reported in Table 5.

The MODE algorithm was able to correct the error introduced in the reflux ratio of the first column.

4.3. Combined SDM-MODE design procedure

The integration between the SDM and the MODE algorithm appears to be certainly a powerful tool for the optimal design of distillation sequences and a closer integration between the methods is now considered. The aim of the integration is the reduction of the computational time avoiding at the same time, the possibility of design errors propagation between the SC sequence and the alternative configuration.

According to the flowchart of Fig. 6 once the connection between the distillation sequence and the correspondent SC sequence is identified, the reference SC sequence is designed following the

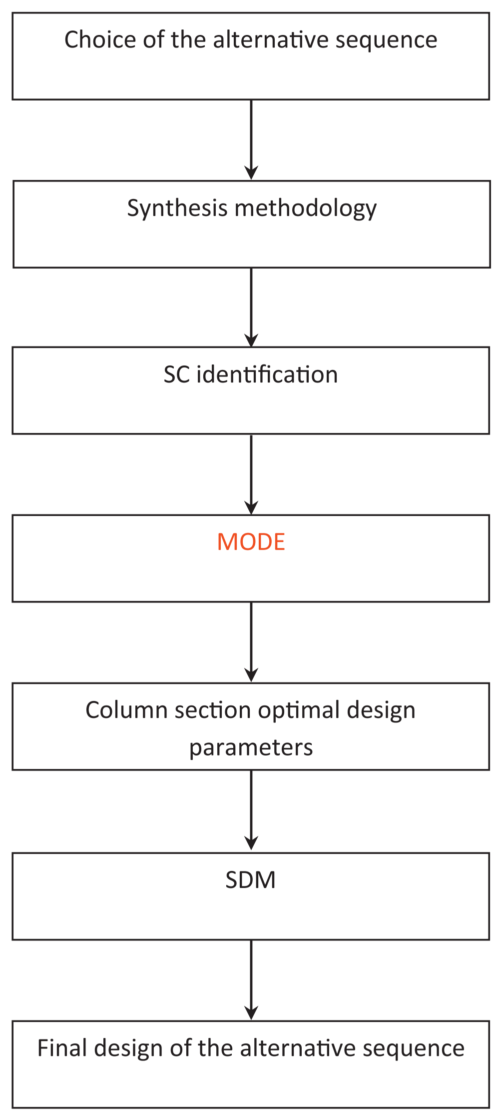

Fig. 6. Hybrid MODE and SDM design procedure.

Table 7
Design parameters, energy consumption and capital costs of the MSC of Fig. 2(d) obtained with the hybrid MODE and SDM.

	C1	C2	C3
N	50	68	41
N_F	32	35	16
P_C (bar)	1.6	1.0	1.0
N_s	–	51	–
D (kmol h^{-1})	35.00	10.10	9.90
B (kmol h^{-1})	65.00	4.70	40.30
S (kmol h^{-1})	–	50.20	–
RR	0.89	12.06	10.37
Φ (m)	0.72	1.33	1.04
ΣQ_c (kW)		−2585.62	
ΣQ_r (kW)		2672.29	
CC ($ yr^{-1})		295540	
TAC ($ yr^{-1})		1643878	
η		12.85	

traditional procedure that includes the short-cut design followed by a rigorous simulation. Then the SC design is used to initialize the MODE algorithm. This step avoids the possible propagation of design errors. The solution obtained can be considered optimal and a direct parameters transposition with the SDM is possible. In this way it is possible to get the alternative sequence final design. This combined design methodology incorporates the MODE algorithm from the very beginning of the design procedure assuring the effectiveness of the SDM.

In this case the configuration to be optimized is the SC, the optimization problem was reformulated as follow:

$$\min(\text{TAC}),\ \max(\eta)$$

$$= f(N_1, N_{F1}, RR_1, N_2, N_{F2}, RR_2, N_3, N_{F3}, RR_3, N_4, N_{F4}, RR_4) \quad (6)$$

where the number indicates the column in the sequence (from left to right), subject to:

$$y_m \geq x_m \quad (7)$$

$$\text{Limit}_{\text{lower},\ var} \geq x_{var} \geq \text{Limit}_{\text{upper},\ var} \quad (8)$$

Applying this procedure, the final design of the MSC sequence was obtained after 70 h and the parameters are reported in Table 7.

Comparing this result with the previous cases, it is possible to notice the general agreement among the solutions obtained. The difference in the capital costs between the design obtained initializing the MODE algorithm with the SDM and the combined design method, is of about 3%. On the same way, it can be observed that the values of TAC and thermodynamic efficiency are inside the range of 1% of difference compare to those obtained with SDM, and the others MODE-SDM combined methodologies. In this case the combined methodology allows a 28% reduction of the computational time compared to the stand-alone MODE algorithm.

5. Conclusions

The SDM was introduced as a distillation column design method based on the correspondence between the column sections of the SC sequences and the corresponding sections in the alternative sequences performing the same separation task. In this way the design parameters are transposed from the SC design to the corresponding alternative sequence.

On the other hand the MODE algorithm represents an excellent tool to optimize different objective functions by means of the differential evolution stochastic method. The main difference between the methods is that the SDM is based on the linkage between the synthesis procedure and the design, the MODE instead, has a strong mathematical basis not related to the specific case. Both methods suffer different benefits and drawbacks. The SDM is fast but there is the possibility to propagate the design errors from the SC to the alternative sequences, the MODE algorithm is mainly too slow. The combination of the design methods was explored as their natural evolution to get a fast and reliable combined design method. A five-component mixture was considered and a specific distillation sequence was selected as alternative to the classic SC sequences. The alternative sequence chosen for the design belongs to the category of modified simple column (MSC) sequences, where each product is obtained as a distillate or as a residue.

First it was proved that the MSC sequence has 9% reduction in the total condenser and reboiler duty together with 9% saving in the capital cost, compared to the corresponding SC. Then the SDM and the MODE design methods were used to get the sequence's configuration parameters. Similar solutions were obtained regarding the energy consumption with analogous and relatively high values of the thermodynamic efficiency, but a consistent difference in the capital cost was evidenced, and as a consequence a moderate difference in the TAC. The design obtained applying the SDM has a capital cost that is 37% and a TAC 7.5% less than the value obtained with the MODE algorithm.

Two different possible combination methods between the design methods have been considered. In the first one, the MODE algorithm was simply initialized by the design parameters obtained with the SDM. The computational time, for the case considered, was reduced of about 39% compare to the stand-alone MODE algorithm and the solution obtained is still the optimal one. In the second possible integration, the MODE algorithm was considered at the beginning of the synthesis procedure optimizing the SC reference sequence. Then the SDM was used to quickly get the design of the alternative sequence. This type of integration avoids the possibility of the propagation of overestimate design parameters when the SDM is directly used to move from the SC to the alternative sequence. In this last case the reduction of the computational time was 28% compared to the stand-alone MODE algorithm, mainly because of the higher number of decision variables associated to the SC sequences. Anyway the possibility of error propagation was decreased. The results obtained proved that this type of integration is able to reduce the drawbacks of the single design methods.

Moreover, these results show a general conclusion when is more suitable to use an optimizer as the MODE for tuning the configuration's design obtained by the SDM, and when it could be more appropriate to integrated MODE since the beginning of the design procedure. When the number of decision variables in the reference SC sequence is high, the initialization of the MODE algorithm with the SDM can lead to the final solution in a reasonable time, with still the possibility to overcome some errors propagated through the SDM procedure.

On the other hand, if the number of decision variable of the SC reference sequence and the corresponding alternative sequence is not so different, then the MODE algorithm could be integrated before the synthesis of the final SDM sequence without any extra computation effort and avoiding any possible error propagation.

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