

Multiobjective Optimization Approach for Integrating Design and Control in Multicomponent Distillation Sequences

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ABSTRACT: This work introduces a multiobjective optimization approach to integrate the design and control of multicomponent distillation sequences. The evaluation of the control properties and the design of the distillation systems were evaluated through the calculation of the condition number and the total annual cost of each design, respectively. Three distillation systems, including the direct sequence, the indirect sequence, and the dividing wall column along with three mixtures with representative ease of separation index (ESI) values and three different feed compositions, were studied. In addition, in a posterior stage to the optimization process, the Eco-indicator 99 for each design was estimated to quantify the environmental impact of the distillation systems. The results offer the trade-offs between the control properties and the design, which is shown through Pareto optimal solutions that enable selection of the solutions that establish the proper balances between both objectives.

1. INTRODUCTION

Historically, and also common today, the chemical process design and the evaluation of the control properties are two problems approached and solved in a separated and sequential way. In a first stage, the process is designed in order to achieve the aims of the design (e.g., the product specifications that meet the requirements of the markets), and in a second stage the control aspects are analyzed and solved. This sequential methodology may present some deficiencies such as dynamic constraint violations, process overdesign, or underperformance, and a robust performance is not guaranteed.¹ Another disadvantage is related to the way in which the process decisions influence the control operation of the process; in a realistic scenario stated by a competitive market, the chemical processes must operate as flexibly as possible in order to adapt in an adequate way to the changes in the product specifications, the demand of consumers, and the variations in the raw materials. In this context, the utilization of appropriate strategies for integrating design and control would allow the suitable operation of the process by improving the profitability through the increment of the throughput production and also the increment in the yield of high value products, besides the minimization in the energy consumption, pollution, and as a direct consequence the environmental impact. Therefore, the development of the idea of integrating design and control may produce significant economic benefits in addition to improvements in the operation of processes through the incorporation of the assessment of the process dynamics in the initial stages of the design. These interactions between the design and control have been documented in past decades.^{2–8} The ideas developed in these works have triggered some of the literature to sketch a general methodology for integrating design and control based on different methods to assess the dynamic properties of the design, for example index-based methods,^{9–11} dynamic optimization-based methods,^{12–16} robust metrics-based methods,^{17–22} and recently probabilistic-based methods.²³ Most of

these methodologies approach the integration of design and control; however, only a few have been applied to the simultaneous integration of large scale process such as multicomponent distillation systems.

In general, the integration of design and control becomes an optimization problem that represents a significant computational burden. Therefore, global optimization methods are desirable in order to solve this problem. These methods can be classified as deterministic global optimization methods and stochastic global optimization methods; the first class offers a guarantee of finding the global optimum of the objective function, provided that the objective function is convex. However, strategies in this class often require high computational time (generally more time than stochastic methods) and, in some cases, a problem reformulation is needed. The use of rigorous design and thermodynamic models leads to very large nonconvex models, which are very difficult to converge. Moreover, taking into account structural and design decisions leads to the inclusion of integer variables, further increasing the difficulty of solving the model. Finally, additional convergence problems are generated when discontinuous functions, such as complex cost functions, are introduced in the model. Recently, some deterministic methodologies that integrate design and control have been developed.^{24–26} On the other hand, stochastic global optimization methods allow obtaining good solutions in moderate computational time. In addition they are very flexible to implement and easy to use, and additional transformations of the original problem are avoided. This is particularly interesting because medium and large scale optimization problems can be implemented in a reasonable computational time. One of the stochastic methods that has

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received considerable attention is differential evolution (DE),²⁷ which was first introduced for solving single objective optimization problems over a continuous domain. Recently, Srinivas and Rangaiah²⁸ have proposed an improvement to the usual DE steps: it consists of the inclusion of the concept of tabu search.²⁹ The tabu algorithm allows keeping a record of recently visited points to avoid further revisiting of explored areas. In particular, Srinivas and Rangaiah²⁸ utilized the concept of a tabu list (TL) with DE, which avoids revisiting points or solutions during the optimization process and reducing this way the computational time. This algorithm was improved by Sharma and Rangaiah,^{30,31} and it was identified as MODE-TL (Multi-Objective Differential Evolution with Tabu List); in this way, this algorithm is capable of dealing with multiobjective optimization problems, in particular with large scale chemical engineering optimization problems.^{32–35} It should be noticed that a multiobjective methodology is highly desirable in a design and control integration approach as the trade-offs between controllability and design aspects can be established.

Therefore, in this paper is presented a multiobjective optimization approach for multicomponent distillation sequences integrating design and control issues. The controllability is evaluated through the calculation of the condition number of the decomposition of the relative gain matrix of the distillation systems in an operating nominal point, whereas the design is evaluated through the estimation of the total annual cost of the distillation sequences studied; namely, these are the objective functions to be simultaneously minimized in the multiobjective optimization approach. This paper is organized as follows: section 2 provides the formulation of the multiobjective optimization design and control integration problem, section 3 shows the case studies, section 4 presents the results and the discussion, and finally section 5 presents the conclusions.

2. FORMULATION OF THE MULTI-OBJECTIVE OPTIMIZATION PROBLEM OF DESIGN AND CONTROL OF DISTILLATION SEQUENCES

The integration of design and control in multicomponent distillation systems leads to a large scale optimization problem. Therefore, the aim of this paper is to introduce a suitable optimization strategy for simultaneously relating both objectives (design and control). In this work, the condition number has been established as the index to evaluate the controllability properties; the condition number has been utilized as a qualitative assessment of the control properties of a design.^{9,36–38} The calculation of the condition number has been carried out through the singular value decomposition of the relative gain matrix of the design in the nominal point, e.g., for the design that fulfills the restrictions, previous to the calculation of the condition number, the singular values are obtained. For example, consider the mathematical expression eq 1, which represents the relative gain matrix of a linear system.

$$K = W\Sigma V^T \quad (1)$$

where W and V are unitary matrixes and Σ is a matrix whose diagonal elements are the singular values σ . Assuming that K is not singular, then the condition number of K , γ , is a positive number which relates to the minimum singular value, σ_* , and the maximum singular value, σ^* , being neither of these two zero. The condition number, γ , can be estimated as in eq 2:

$$\gamma = \frac{\sigma^*}{\sigma_*} \quad (2)$$

Large values of σ_* and small values of σ^* are desirable so that the process may assimilate the perturbations without system destabilization.⁶ Therefore, lower values of the condition number of a design are preferable over upper values. In this study the condition number of the relative gain matrix obtained in an open loop control strategy for each design is estimated by generating the relative gain matrix in a nominal state of each distillation sequence design. The elements of this matrix are calculated through the introduction of perturbations in the manipulated variables, which are the reflux ratio and the reboiler duty for the conventional sequences studied, and the reflux ratio, the reboiler duty, and the sidestream molar flow rate for the thermally coupled dividing wall distillation column (see Figure 1). The magnitude of the perturbations was defined as a 0.5% positive change in the values of the manipulated variables in the nominal state; the level of these perturbations is low enough that it is assumed the response of the system can be approached as a first order response. It is very important to note that the gain matrix is scaled to take into account variations of different orders of magnitude of the perturbations.

One drawback of the singular value decomposition is the fact that the singular values depend on the system of units used. Applying the singular value decomposition to relative gain matrix will include the effects of such units; therefore, it is important to use a scaling method to remove this dependency and provide reliability in the results as well as a physical meaning. In order to approach this issue, some authors (see, for instance, refs 6, 39, and 40) have proposed scaling methods for the manipulated variables and the control variables. For the distillation sequences in this study there are three important control variables; such variables are the molar purities of each of the components of the corresponding ternary mixture, and these are naturally bounded between 0 and 1. Manipulated variables are used for each distillation sequence; they are the reflux ratio and the reboiler duty for the conventional sequences, and the reflux ratio, the reboiler duty, and the sidestream molar flow rate for the dividing wall distillation column. These manipulated variables have units and are not bounded naturally. To eliminate this drawback, it is proposed to limit the manipulated variables considering that the maximum aperture that can reach the control valves is twice the nominal value of the steady state; therefore, in principle the valves are open to 50%. This implies that, for the relative gain matrix, the step change is implemented in the manipulated variable to be divided by twice the steady state to have the same range of variation in both the closing and opening operations of the control valves. This allows for a physical interpretation to the way of scaling of the manipulated variables, to link the amount of change of the manipulated variables with the magnitude of change of the position of the corresponding valve stem, which can only vary between 0 and 100% open (0 and 1). With this form of scaling it is achieved simultaneously dimensionless standardization and manipulated variables; the term $(1/2)p$ has been included in eq 3 in order to achieve this purpose.

In the case of distillation columns, the selection of manipulated variables, for perturbation in the gain matrix, are fairly well established and used successfully in practice, at least for conventional columns. Typically on a distillation column there are four control handles: distillate flow rate, reflux flow

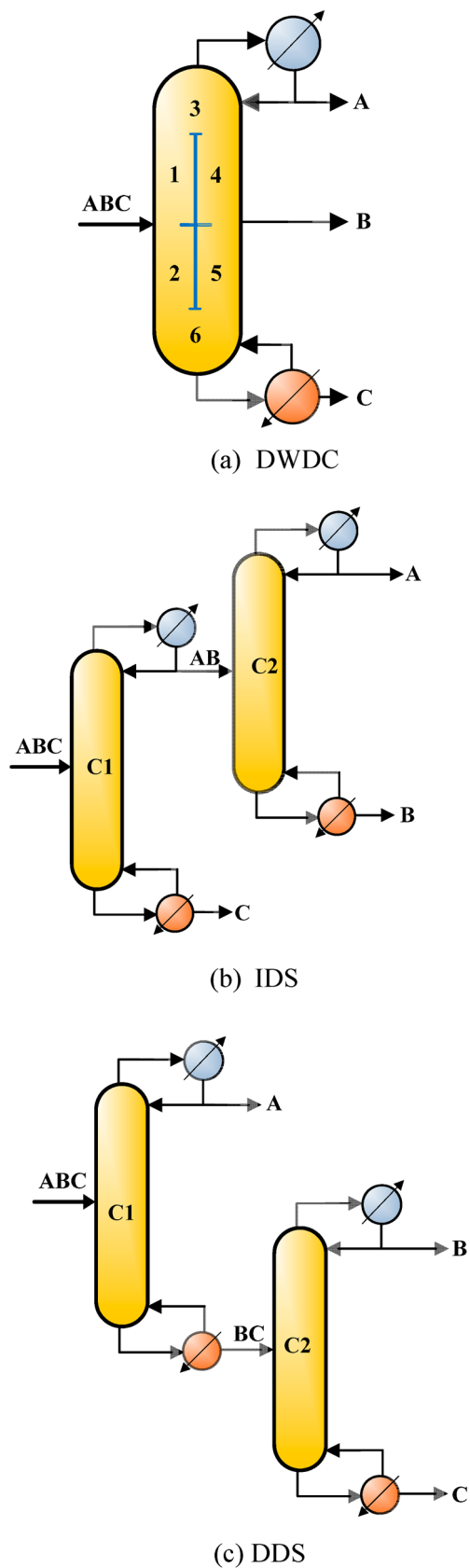


Figure 1. Studied distillation sequences: (a) DWDC, dividing wall distillation column; (b) IDS, indirect distillation sequence; (c) DDS, direct distillation sequence.

rate, bottoms flow rate, and the heat rate into the reboiler. However, material balance usually dictates two of these handles must be used to control the level in the accumulator tank and the level in the base of the column. That leaves only two variables which can be manipulated, e.g., the reflux ratio. This, and other meaningful ratios, can be used to replace the direct manipulation of the four control handles. The reflux ratio and the heat rate into the reboiler (reboiler duty) have been found as some of the best manipulated variables in control studies (see, for instance, refs 41 and 42). Equation 3 represents the relative gain matrix for the direct distillation sequence.

$$\begin{bmatrix} K_{11} & K_{12} & K_{13} \\ K_{21} & K_{22} & K_{23} \\ K_{31} & K_{32} & K_{33} \end{bmatrix} = \begin{bmatrix} \frac{x_A^{R_1} - x_A^{SP}}{(1/2)p} & \frac{x_A^{R_2} - x_A^{SP}}{(1/2)p} & \frac{x_A^{Q_2} - x_A^{SP}}{(1/2)p} \\ \frac{x_B^{R_1} - x_B^{SP}}{(1/2)p} & \frac{x_B^{R_2} - x_B^{SP}}{(1/2)p} & \frac{x_B^{Q_2} - x_B^{SP}}{(1/2)p} \\ \frac{x_C^{R_1} - x_C^{SP}}{(1/2)p} & \frac{x_C^{R_2} - x_C^{SP}}{(1/2)p} & \frac{x_C^{Q_2} - x_C^{SP}}{(1/2)p} \end{bmatrix} \quad (3)$$

The elements in the left side of eq 3, K_{ij} , are the relative gain matrix. Moreover, the elements of the first row in the right side correspond to the differences among the molar purities of component A in the nominal state, x_A^{SP} , and the molar purities after the perturbations, p , are introduced, $x_A^{R_1}$ is the molar purity of component A after the perturbation of the reflux ratio in column 1, $x_A^{R_2}$ is the molar purity of component A after the perturbation of the reflux ratio in column 2, and $x_A^{Q_2}$ is the molar purity of component A after the perturbation of the heat duty of column 2. Notice that these last two perturbations do not affect the molar purity of component A; therefore, the elements of the second and third columns in the first row are zero. This situation makes the solution of the mathematical problem easy.

In order to integrate design and control in multicomponent distillation systems, in this work the design evaluation is assumed to be done through the total annual cost estimation, so that the total annual cost, TAC, and condition number, CN, integrate design and control. The objective function that includes the total annual cost and the condition number for the distillation sequences can be mathematically expressed as in eq 4:

$$\min Z = \{TAC; CN\} \quad (4)$$

$$TAC = f(N_S, C_d, R_a, C_a, h_u, c_o)$$

$$CN = f(\sigma_*, \sigma^*)$$

subject to

$$\vec{y}_{i,PC} \geq \vec{x}_{i,PC}$$

$$\vec{w}_{i,FC} \geq \vec{u}_{i,FC} \quad (5)$$

The objective function indicates that the total annual cost and the condition number are simultaneously minimized during the optimization process; the total annual cost of a distillation sequence depends on the number of stages N_S , column diameters C_d , area of condensers C_a , area of reboilers R_a , heating utilities h_u and cooling utilities c_o , whereas the condition number relates the minimum singular value σ_* and the maximum singular value σ^* . The objective function is restricted to the fulfillment of the purity vectors and the molar

flow rate vectors for the components in the mixture; e.g., the values of the purities for the components obtained during the optimization process $\bar{y}_{i,PC}$ must be either greater than or equal to the specified values of purities for the components $\bar{x}_{i,PC}$. Furthermore, the molar flow rates $\bar{w}_{i,FC}$ obtained must also be either greater than or equal to the specified values of the molar flow rates $\bar{u}_{i,FC}$. The decision variables in the optimization process for the studied distillation sequences (see Figure 1) are eight variables among integer and continuous for the direct and the indirect distillation sequence, namely the total number of stages, N_s , feed stage, F_s , reflux ratio, r , and reboiler duty Q_c of each column. The dividing wall distillation column requires 11 decision variables among integer and continuous. These variables are the following: total number of stages of the prefractionator, N_p , feed stage of the prefractionator, F_p , total number of stages of the main column, N_c , liquid and vapor interconnection stages N_l and N_v , respectively, stage of withdrawal of sidestream product, N_w , vapor interconnection flow rate, V_β , liquid interconnection flow rate, L_β , sidestream product flow rate S_β , reflux ratio, r_p , and heat duty of the column Q_p . It is important to notice that the dividing wall distillation column has been modeled as the Petlyuk column;^{43–46} therefore, this is the reason for the existence of the variables N_l and N_v .

The multiobjective optimization problem states an important degree of difficulty so that a suitable optimization strategy must be used. In this work, the multiobjective optimization hybrid method has been used, namely the Multi-Objective Differential Evolution with Tabu List algorithm (MODE-TL).³⁰ In the MODE-TL (see the flowchart given in Figure 2) a population of NP individuals is randomly initialized inside the bounds on decision variables. Then, values of the objectives and constraints are calculated for each individual of the initial population. The TLS (tabu list size) is half the population size, and the tabu list (TL) is randomly filled with 50% individuals of the initial population; initial individuals are also identified as target individuals (i). A trial individual is generated for each target individual by mutation and crossover on three randomly selected individuals from initial/current/parent population. The elements of the mutant vector compete with those of the target vector, with a probability Cr to generate a trial vector. A tabu check is implemented in the generation step of the trial vector of the MODE-TL,^{30,31} and the trial individual is generated repeatedly until it is away from each individual in the TL by a specified distance called the tabu radius (Tr). Euclidean distance between trial individual and each individual in TL is calculated in the normalized decision variable space for accepting the trial individual. After that, objectives and constraints are calculated for the temporarily accepted trial individual. The trial individual is stored in the child population and added to TL. After generating the trial individuals for all the target individuals of the current population, nondominated sorting of the combined current and child populations followed by crowding distance calculation, if required, is performed to select the individuals for the next generation (G).^{30,31} The best NP individuals are used as the population in the subsequent generation. For further details about the MODE-TL, the reader is referred to the work by Sharma and Rangaiah.³⁰

The implementation of the global optimization approach involved a hybrid platform which linked Aspen Plus, Microsoft Excel, and Matlab through the implementation of a COM technology (see Figure 3). During the optimization process, a decision vector of design variables is sent from Excel to Aspen

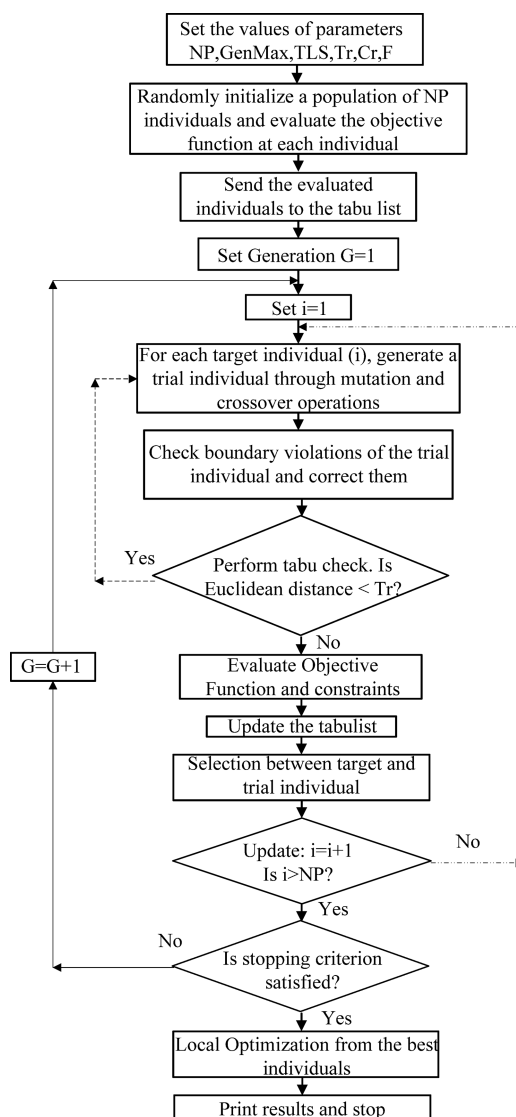


Figure 2. Flowchart of the used multiobjective algorithm.

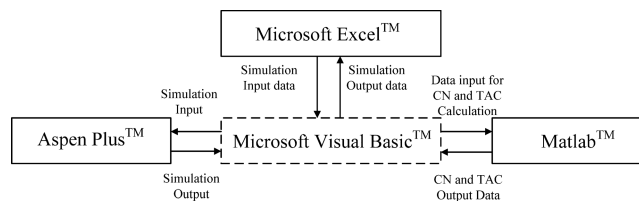


Figure 3. Hybrid platform to implement the multiobjective optimization approach.

Plus; in this process simulator rigorous calculations for the data that identify a particular design of the distillation systems are obtained (e.g., temperature profile, molar composition profile, molar flow profile, etc.) via resolution of phase equilibria along with the complete set of MESH equations by using the RadFrac module. These data are returned from Aspen Plus and stored in Excel; perturbations are applied on the manipulated variables and new simulations are executed. After these simulations are completed, the differences among the components' molar purities in the nominal state and the components' molar purities after the perturbations are estimated. These data along with the necessary data to estimate

the total annual cost are sent from Excel to Matlab. In this software, the calculation of both objective functions is carried out, the values obtained for the objective functions are returned to Excel, and new vectors of design variables are generated according to the stochastic procedure of this method. For the optimization process, in this study the values for the parameters associated with the used MODE-TL³⁰ algorithm are the following: population size (NP), 200 individuals; generations number (GenMax), 200; tabu list size (TLS), 100 individuals; tabu radius (Tr), 2.5×10^{-6} ; crossover fractions (Cr), 0.8; mutation fractions (F), 0.6. These values were obtained from the literature.³⁰

3. CASE STUDIES

In this study three ternary mixtures containing hydrocarbons (Table 1) with representative values of the ease of separation

Table 1. Mixtures Analyzed

mixture	component	$\alpha_{A,B}$	$\alpha_{B,C}$	ESI
M1	<i>n</i> -propane (A)	3.28	3.05	1.07
	<i>n</i> -butane (B)			
	<i>n</i> -pentane (C)			
M2	2-methylpropane (A)	1.36	3.05	0.44
	<i>n</i> -butane (B)			
	<i>n</i> -pentane (C)			
M3	<i>n</i> -butane (A)	2.38	1.28	1.85
	2-methylbutane (B)			
	<i>n</i> -pentane (C)			

index (ESI) as defined by Tedder and Rudd⁴⁷ with three feed compositions (Table 2) were selected in order to study the

Table 2. Feed Composition for Each Mixture

feed composition	molar composition
C1	A = 0.3, B = 0.3, C = 0.4
C2	A = 0.3, B = 0.4, C = 0.3
C3	A = 0.4, B = 0.3, C = 0.3

influence of the separation difficulty of the two main splits for ternary mixtures on the simultaneous design and control approach. The feed flow rate was 100 kmol h^{-1} as saturated liquid, and the specified purities for the product streams were assumed to be 98.7, 98, and 98.6 mol % for A, B, and C, respectively. The design pressure for each separation was chosen to ensure the use of cooling water in the condensers. Since the feeds involve hydrocarbon mixtures, the Chao–Seader correlation was used for the prediction of the thermodynamic properties. This model is usually recommended for petrochemical plants operating at low or medium pressure.^{48,49} On the other hand, the distillation sequences studied are shown in Figure 1.

4. RESULTS

This section presents the results of the multiobjective optimization method. All the runs were performed on an Intel Core i7-4790 CPU@3.6 GHz, 12 GB computer. The computing time required to obtain the Pareto optimal solutions varied according to the mixture and the distillation sequence: on average each run of the DDS and each mixture and each feed composition required 75.8 h, each run of the IDS and each mixture and each feed composition required 70.5 h; whereas

each run of the DWDC and each mixture and each feed composition required 87.5 h. The estimation of the total annual cost was done through the utilization of the modular method^{50,51} and the available equations in the publication by Turton et al.⁵² Moreover, in a subsequent stage of the optimization process, calculations of the Eco-indicator 99 have been carried out for each of the optimum distillation sequence designs in order to quantify the environmental impact; therefore, the Eco-indicator 99 is not an objective in the optimization process. In the Eco-indicator 99 method each impact category is evaluated according to the individual scores;⁵³ this method has been used for environmental impact quantification purposes of several chemical processes.^{54–56}

The Pareto optimal solutions for mixture 1 with ESI = 1.07 and feed compositions 1, 2, and 3 are shown in Figure 4. It is

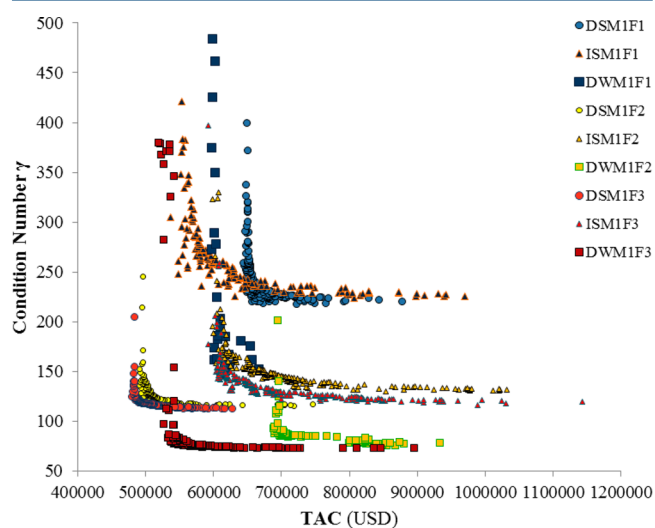


Figure 4. Pareto front for mixture 1 and feed compositions 1–3.

possible to determine that, for all the feed compositions, the dividing wall column (DWDC) offers most of its designs with lower condition number values compared with the CN values of the designs for the direct sequence (DDS) and the indirect sequence (IDS). Therefore, the DWDC shows the best control properties in all the feed compositions. Nevertheless, the compromises between both objectives, TAC and CN, can be established for all the sequences in this mixture. For example, for feed composition 1, the IDS shows some of its designs with TAC slightly lower than the DWDC, and also the IDS offers most of their designs with lower TAC with respect to the direct sequence. For practical purposes, the DWDC provides good designs with CN values between 150 and 200 and TAC values from \$600,000 to \$700,000. On the other hand, for feed composition 2, the DDS provides good designs with the lowest TAC in comparison with the IDS and the DWDC but this last offers most of its designs with CN under a value of 100, so the DWDC presents the best control properties. However, most of these designs have a greater TAC compared with the designs of the IDS; nevertheless the IDS offers many of the designs with the highest values of CN. For composition 3, the DDS offers the designs with the best TAC compared with the IDS and the DWDC. However, the DDS shares designs with similar CN values with the IDS but none of these design sequences are better in control properties than the DWDC. In general, the DWDC offers designs with good control properties for all the

Table 3. Design Variables of the DDS, IDS, and the DWDC for Mixture 1 and Feed Compositions 1–3

	DDS		IDS		DWDC			
	C1	C2	C1	C2	sections 1 and 4	sections 2 and 5	section 3	section 6
Feed Composition 1								
no. of stages	21	40	22	22	14	5	18	12
feed stage	17	35	13	16	–	32	–	–
reflux ratio	6.8	5.7	1.7	4.1	–	–	9.9	–
top pressure, bar	15	8	10	16	–	–	16.3	–
diameter, m	0.77	0.74	0.74	0.6	–	–	1.3	–
sidestream stage	–	–	–	–	29	–	–	–
reboiler duty, kW	572.13	390.44	598.69	361.44	–	1333.75	–	–
CN	220.3		236.1		–	147.6	–	–
TAC	664 312.9		581 434.6		–	610 647.1	–	–
Feed Composition 2								
no. of stages	19	18	25	20	24	6	18	3
feed stage	12	12	21	18	20	–	–	–
reflux ratio	3.2	1.5	1.3	2.5	–	–	4.6	–
top pressure, bar	15.8	4.7	9.3	9.3	–	–	16	–
diameter, m	0.64	0.69	0.73	0.45	–	–	1.3	–
sidestream stage	–	–	–	–	28	–	–	–
reboiler duty, kW	496.58	394.46	767.66	370.9	–	679.58	–	–
CN	120.3		161.2		–	87.7	–	–
TAC	512 184.6		629 376.9		–	689 391.9	–	–
Feed Composition 3								
no. of stages	17	16	17	23	14	6	12	9
feed stage	8	12	13	20	–	–	12	–
reflux ratio	2.1	2.03	2.2	1.6	–	–	3.5	–
top pressure, bar	16	4.8	15.9	15.9	–	–	15.9	–
diameter, m	0.7	0.55	1.1	0.57	–	–	1.7	–
sidestream stage	–	–	–	–	18	–	–	–
reboiler duty, kW	515.01	324.85	770.04	383.74	–	718.61	–	–
CN	121.1		141.7		–	78.9	–	–
TAC	487 068.7		609 857.8		–	538 032.1	–	–

feed compositions of mixture 1, but the designs with the best TAC are spread between the IDS and the DDS. Therefore, multiple designs show the compromises between the TAC and CN. Table 3 shows the design variables of the distillation sequences that exhibit the lowest CN and TAC values of each design for all the feed compositions. These designs are taken from the curve zone of the Pareto optimal solutions shown in Figure 4. It is important to note that the dividing wall distillation column has been modeled as the Petlyuk column; the depiction of the sections and the determination of the number of stages for each of these sections are explained precisely in this modeling.⁵⁷ For example, the number of stages of section 3 contains the stages from the top of the main column to the liquid flow rate interconnection stage, whereas section 6 contains the number of stages from the bottom of the main column to the vapor flow rate interconnection stage. On the other hand, the number of stages for section 4 is determined by counting the existing stages from the liquid flow rate interconnection stage to the sidestream product flow rate stage of the main column. Finally, the number of stages for section 5 contains the stages from the sidestream product flow rate stage to the liquid flow rate interconnection stage.

Values of the energy consumption, Q , of the optimal designs are shown in Figure 5; it is possible to link the energy consumption of each design and its control properties in this figure. It should be noticed that the DWDC offers significant energy savings for feed compositions 2 and 3. This behavior of the DWDC has been reported in sequential methodologies for

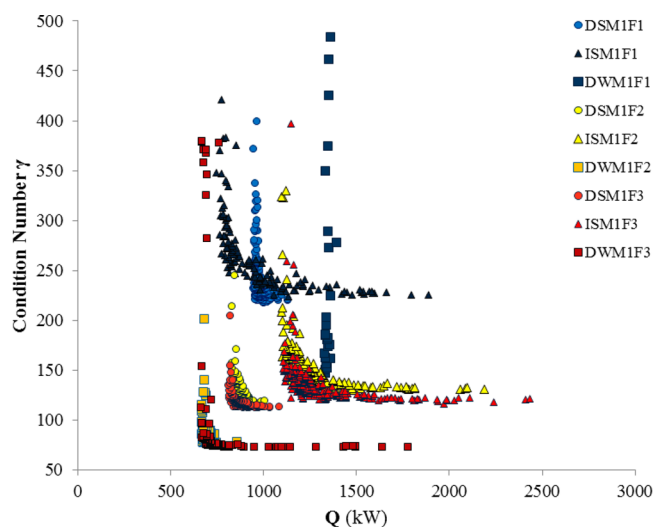


Figure 5. Energy consumption and condition number for mixture 1 and feed compositions 1–3.

design and control, where there was stated that the DWDC offers significant energy savings with respect to the conventional distillation arrangements.^{58,59} The Eco-indicator 99 and the CN values for the optimal designs are presented in Figure 6. According to these results it is possible to identify the designs for the distillation sequences that show the lowest and largest environmental impacts, so it is also possible to establish the

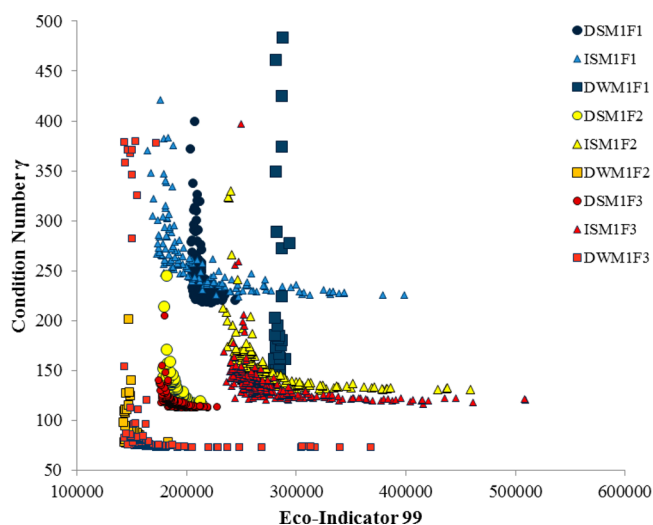


Figure 6. Eco-indicator 99 and condition number for mixture 1 and feed compositions 1–3.

relationships between the control properties of the designs and the environmental impact.

The second mixture with $ESI = 0.44$ contains two linear hydrocarbons and one isomer; three feed compositions were also studied. This mixture states a difficult separation task between two components. For example, for the ternary mixture A, B, C (see Table 1), the values for the relative volatilities of two adjacent components are very close. These components are 2-methylpropane and *n*-butane; therefore, the difficult separation task is found in the split A/B. This mixture has been included in order to study the effect of the separation task A/B on the design and control integration approach. Figure 7 shows

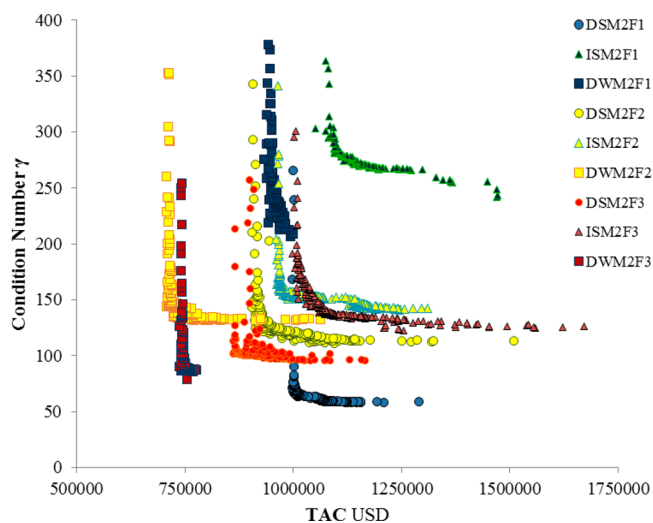


Figure 7. Pareto front for mixture 2 and feed compositions 1–3.

the Pareto optimal solutions obtained for this mixture. Interesting results may be found for this mixture: in the feed composition 1, the DDS offers the designs with the best CN values, the DWDC shows the intermediate best designs with respect to the CN, and the IDS offers the designs with the poorest control properties. In terms of cost, the DWDC presents the designs with low TAC while the DDS and the IDS offer designs with similar TAC. The behavior of the sequences for feed composition 2 allow determining that the DDS shows

the designs with the best CN, while the DWDC and IDS contain designs with similar CN; with respect to the TAC, the DWDC presents the best designs and the IDS and DDS offer designs with similar TAC. In feed composition 3, the DWDC and the IDS are the sequences that offer the designs with the low CN values and the DDS shows the designs with the highest CN. The DWDC presents many of its designs with the lowest TAC. In general, for this mixture the DDS offers good designs with low CN while the DWDC shows the designs that provide the lowest TAC and the IDS presents the designs that may compensate both objectives, being this sequence the one that does not provide designs as good as the DWDC and the DDS.

The energy consumption for the optimal solutions and the relationships with the condition number values are shown in Figure 8. It is clear to see that the DWDC presents designs that

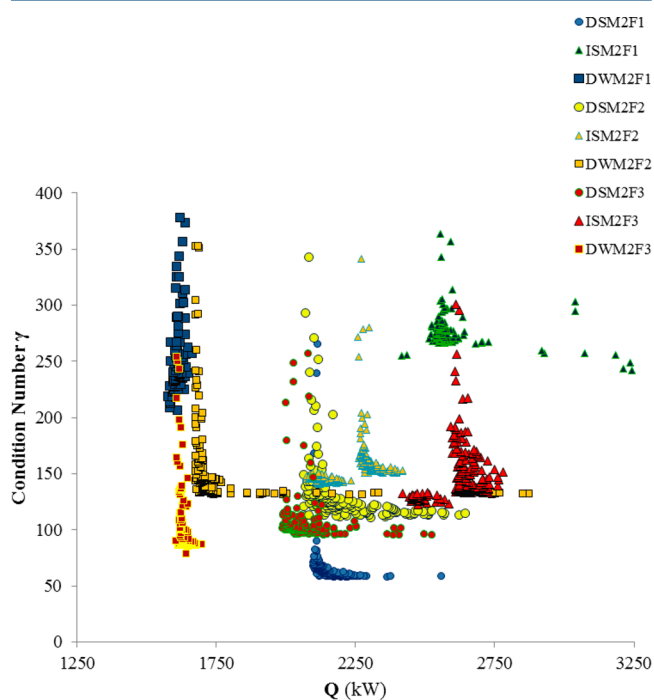


Figure 8. Energy consumption and condition number for mixture 2 and feed compositions 1–3.

provide substantial energy savings with respect to the IDS and DDS. Moreover, Figure 9 shows the Eco-indicator 99 values for the optimal designs; these results are consistent with the energy consumption results as this factor is one of the individual categories that has a larger impact in the Eco-99 methodology. Therefore, the DWDC offers the designs with the minimum Eco-indicator 99 values for all the feed compositions, while the DDS shows the designs with intermediate Eco-indicator 99 values and the IDS provides the designs with the largest Eco-indicator 99 values.

The third mixture with $ESI = 1.85$ states a difficult task represented by the split B/C in order to separate 2-methylbutane and *n*-pentane, because the relative volatilities of these components are very close. The Pareto optimal solutions for this mixture and all the feed compositions are shown in Figure 10. It is clear to see that the DWDC offers the designs with the best CN; in other words, good control properties are exhibited by these designs. In addition, the TAC values of the DWDC are significantly lower than the TAC values of the IDS and the DDS. On the other hand, it is

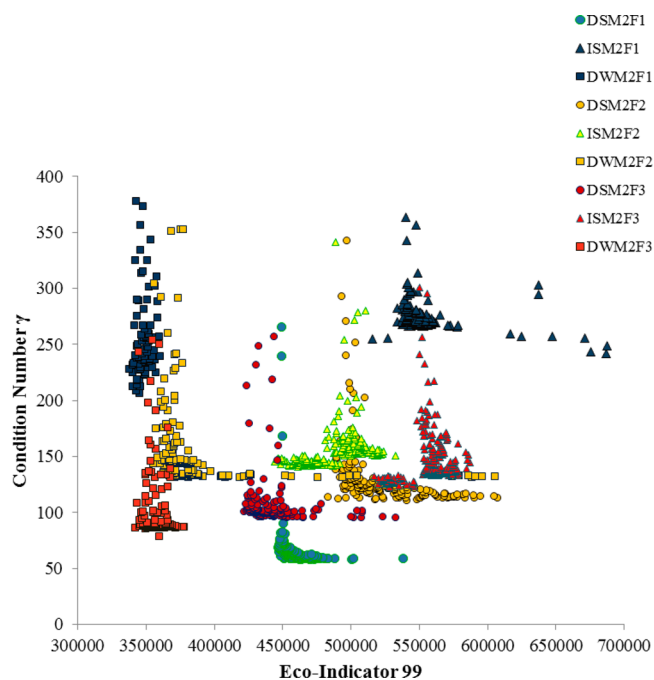


Figure 9. Eco-indicator 99 and condition number for mixture 2 and feed compositions 1–3.

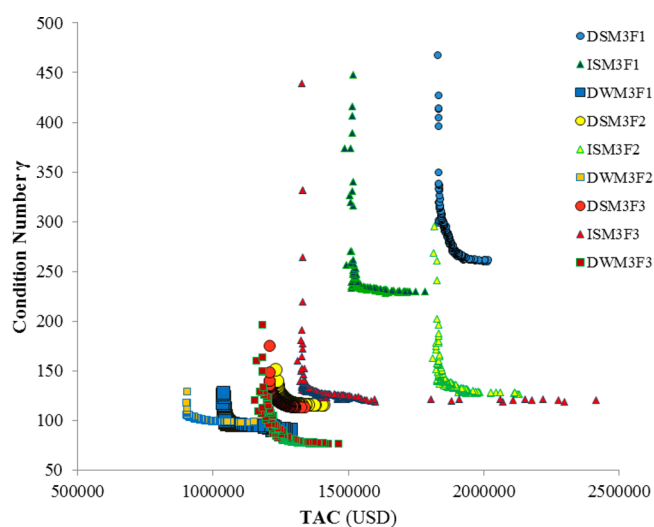


Figure 10. Pareto front for mixture 3 and feed compositions 1–3.

possible to establish the compromises between the TAC and the CN for all the designs of the DWDC, the IDS, and the DDS. Figure 11 shows the energy consumption of each design of the Pareto optimal solutions; it is possible to establish that the DWDC shows considerably lower energy consumption than the IDS and the DDS for all the feed compositions. In addition, the Eco-indicator 99 values of each design are presented in Figure 12 so that these results are consistent with the energy requirements; therefore, the DWDC offers the designs with the lowest environmental impact.

The obtained results in this simultaneous design and control approach show that most of the designs of the DWDC for all the mixtures and for each feed composition exhibit better control properties than the IDS and the DDS; this behavior (i.e., the thermally coupled distillation column shows good control properties) has also been documented in previous

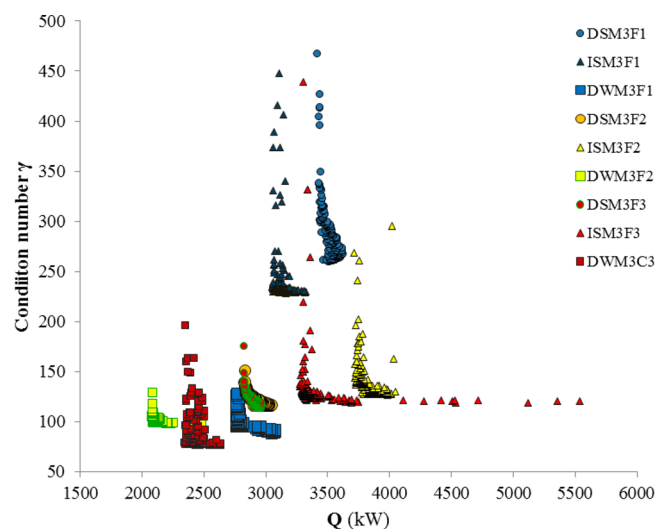


Figure 11. Energy consumption and condition number for mixture 3 and feed compositions 1–3.

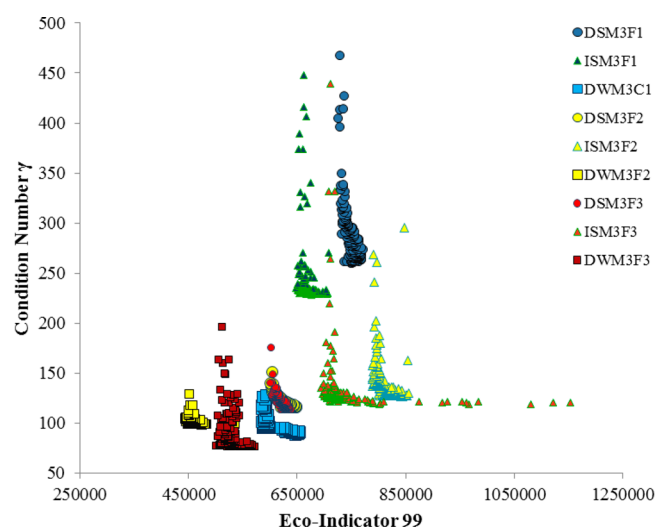


Figure 12. Eco-indicator 99 and condition number for mixture 3 and feed compositions 1–3.

sequential methodologies for design and control of distillation systems for the separation of ternary mixtures.^{60–62} This fact is attributed to the internal interconnections of liquid and vapor in the DWDC and because the remixing of streams is avoided, so the system is less unstable because the gradients in the concentration of species in the mixture tend to be minimized in some regions of the column. In addition, the DWDC shows the designs with the lowest energy consumption, which is consistent with the fact that the existence of internal interconnections favors this condition. In order to summarize the results of this study, Table 4 shows a representation of the results, which has been done through a visual inspection of the Pareto optimal solutions.

The summary of the results for each ESI value can be stated as follows:

Mixture 1 with $ESI \approx 1$. The results show that for this ESI value and all the feed compositions there is no highlighted distillation sequence but the designs with low TAC values are spread among the IDS, the DDS, and the DWDC. On the other

Table 4. Summary of the Obtained Results

	TAC	CN, γ	Q (kW)	Eco-99
mixture 1, ESI \approx 1				
C1	DDS > DWDC > IDS	IDS > DDS > DWDC	DWDC > DDS > IDS	DWDC > DDS > IDS
C2	DDS > IDS > DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC
C3	IDS > DWDC > DDS	IDS > DDS > DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC
mixture 2, ESI < 1				
C1	IDS > DDS > DWDC	IDS > DWDC > DDS	IDS > DDS > DWDC	IDS > DDS > DWDC
C2	IDS > DDS > DWDC	IDS > DWDC > DDS	IDS > DDS > DWDC	IDS > DDS > DWDC
C3	IDS > DDS > DWDC	IDS > DDS \approx DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC
mixture 3, ESI > 1				
C1	DDS > IDS > DWDC	DDS > IDS > DWDC	DDS > IDS > DWDC	DDS > IDS > DWDC
C2	IDS > DDS > DWDC	IDS \approx DDS > DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC
C3	IDS > DDS \approx DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC	IDS > DDS > DWDC

hand, the DWDC offers the designs with the best condition number values.

Mixture 2 with ESI < 1. This ESI value tends to favor the designs for the DWDC with respect to the TAC for all the feed compositions. Moreover, it can be established that the DDS shows the best CN values for the majority of the feed compositions.

Mixture 3 with ESI > 1. The DWDC offers for all the feed compositions the best designs in terms of the TAC and CN values; this ESI value favors considerably the thermally coupled distillation column.

In general, it can be established that the control properties and the total annual cost (where the design variables of the process are associated) are variables in competition. Some authors⁶³ have established that in distillation columns the designs with the minimum operational costs exhibit the worst control properties and as the designs move away from the optimum total annual cost the control properties are improved. It has been explained due to that, in the optimal design for the total annual cost, the design variables are restricted and it can be unfavorable for the dynamic behavior of the distillation column. This is observed in the Pareto optimal solutions obtained in this work.

5. CONCLUSIONS

This paper has introduced a multiobjective optimization approach that integrates the design and control of multi-component distillation sequences. Three distillation sequences and three hydrocarbon mixtures with representative ease of separation indexes and three feed compositions were studied. As reported in previous sequential methodologies that have evaluated the design and control, it has been found in this approach that the dividing wall distillation column exhibits better control properties than the conventional separation systems. Moreover, the results offer the trade-offs between the control properties and the design illustrated through the Pareto optimal solutions that enable selection of the solutions for all the sequences that establish the proper balances between both objectives. In addition, the environmental aspects of the designs, in particular their environmental impacts together with their control properties, can be established.

■ APPENDIX A. DETAILS FOR THE CALCULATION OF TAC

In this work, the total annual cost of each sequence has been estimated as follows:

$$\text{TAC} = \frac{\text{capital cost}}{\text{time of investment}} + \text{operating cost}$$

In the case of the DWDC, this has been modeled as its thermodynamically equivalent the Petlyuk column, and the estimation of the capital cost of the DWDC has been carried out by determining the summation of the cost of the prefractionator and the main column. Specifically, the capital cost of each sequence was calculated by using the modular method^{50,51} and the equations and parameters found in the publication by Turton et al.⁵² The material for all the equipment was established as carbon steel, and 10 years for the time of investment was considered. The operating cost includes cooling and heating utilities, and 8400 h of yearly operation for each sequence was considered. Furthermore, low-pressure steam (6 bar, 87 psia, 160 °C/320 °F) with a cost of \$7.78/GJ, electrical energy with a cost of \$16.8/GJ, and cooling water received at 20 °C and returned at 30 °C with a unit cost of \$0.72/GJ as utility have been considered.⁶⁴

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Notes

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■ NOMENCLATURE

DSM1F1 = direct distillation sequence mixture 1 feed composition 1
 ISM1F1 = indirect distillation sequence mixture 1 feed composition 1
 DWM1F1 = dividing wall distillation column mixture 1 feed composition 1
 DSM1F2 = direct distillation sequence mixture 1 feed composition 2
 ISM1F2 = indirect distillation sequence mixture 1 feed composition 2
 DWM1F2 = dividing wall distillation column mixture 1 feed composition 2
 DSM1F3 = direct distillation sequence mixture 1 feed composition 3

ISM1F3 = indirect distillation sequence mixture 1 feed composition 3

DWM1F3 = dividing wall distillation column mixture 1 feed composition 3

x_A^{SP} = molar purity of component A in the nominal state

$x_A^{Q_1}$ = molar purity of component A after perturbation of the reboiler duty in column 1

$x_A^{R_2}$ = molar purity of component A after perturbation of the reflux ratio in column 2

$x_A^{Q_2}$ = molar purity of component A after perturbation of the reboiler duty in column 2

x_B^{SP} = molar purity of component B in the nominal state

$x_B^{Q_1}$ = molar purity of component B after perturbation of the reboiler duty in column 1

$x_B^{R_1}$ = molar purity of component B after perturbation of the reflux ratio in column 1

$x_B^{Q_2}$ = molar purity of component B after perturbation of the reboiler duty in column 2

$x_B^{R_2}$ = molar purity of component B after perturbation of the reflux ratio in column 2

x_C^{SP} = molar purity of component C in the nominal state

$x_C^{R_1}$ = molar purity of component C after perturbation of the reflux ratio in column 1

$x_C^{R_2}$ = molar purity of component C after perturbation of the reflux ratio in column 2

$x_C^{Q_2}$ = molar purity of component C after perturbation of the reboiler duty in column 2

p = magnitude of perturbations on the manipulated variables, 0.5%

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