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Integrating metaheuristic methods and deterministic strategies for optimizing supply chain equipment design in process engineering

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ABSTRACT

In recent years, the escalating use of supply chains in process engineering has highlighted the need for efficient regional resource distribution. Traditionally, supply chains are designed through deterministic optimization models. However, these models require significant simplifications to mathematically represent the equipment design in these supply chains because of the complexity and nonlinearity these formulations bring to the problem, often leading to suboptimal solutions. This work proposes a novel methodology integrating deterministic and metaheuristic optimization techniques to address this challenge comprehensively. By combining these methods, the approach optimizes supply chain logistics and equipment design, enhancing overall performance, cost-efficiency, and sustainability. A case study on the polystyrene supply chain in Mexico demonstrates the effectiveness of our strategy, showcasing significant economic, environmental, and operational benefits. Two different schemes were used, a direct separation sequence and an indirect separation sequence. The results show that the direct separation sequence is better both economically and environmentally, due to the high energy consumption of the indirect separation. This integrated approach offers a robust mathematical tool for decision-making, setting a new standard in supply chain optimization.

1. Introduction

In recent years, the utilization of supply chains in process engineering has witnessed a substantial increase, driven by the necessity to effectively meet the demand for specific resources in particular regions (Ravindran et al. 2023; Lim et al. 2021). The deployment of these supply chains has predominantly relied on mathematical programming, employing deterministic optimization models to identify an optimal configuration encompassing resources, equipment, suppliers, and the ultimate destination (Lejarza et al. 2022). However, a notable challenge encountered in the application of these optimization models is the simplification inherent in the design of production or generation equipment for the resources intended for distribution through the proposed supply chains (Pistikopoulos et al. 2021; Emenike and Falcone, 2020). This simplification can introduce complexities in addressing the presented scenario. Solving the supply chain and the associated technology design simultaneously is a mathematically complex problem. This complexity arises from the need to consider numerous variables and constraints that interact in intricate ways, often resulting in large-scale, non-linear, and highly constrained optimization problems. Normally, deterministic mathematical models are created to solve process supply chains. This is due to the different strategies that can be used to reduce computing time and relax some mathematical expressions, which helps to easily find an optimal solution (Gilani et al. 2020).

These strategies include linearization techniques, decomposition methods, and heuristic algorithms, which, while effective, often necessitate simplifications in the equipment design to make the problem tractable. As a result, the detailed modeling of equipment performance and integration within the supply chain may be overlooked or approximated, potentially compromising the accuracy and efficacy of the solution (Garcia and You, 2015). The process of simplifying equipment design in the context of supply chain optimization involves assumptions that can lead to suboptimal decisions. For example, standardizing equipment parameters might ignore specific operational efficiencies or maintenance requirements that could impact the overall performance of the supply chain (Sharifnia et al. 2021). However, this solution could be

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a local optimum and not a global optimum, which would be easier to obtain using a stochastic method. Stochastic methods, which account for randomness and uncertainty in the modeling process, can provide a more comprehensive understanding of the supply chain dynamics and the performance of the associated technologies. By incorporating probabilistic elements, these methods can explore a wider range of potential solutions, thus increasing the likelihood of identifying a global optimum. The metaheuristic optimization techniques, incorporated in this methodology, are particularly adept at navigating complex, high-dimensional search spaces to find near-optimal solutions that deterministic methods might miss. For example, genetic algorithms can simulate the process of natural selection to iteratively improve equipment designs, while simulated annealing can avoid local optimal by allowing occasional suboptimal moves, thus escaping the potential pitfalls of traditional optimization methods. Particle swarm optimization, inspired by social behavior patterns of organisms, can efficiently explore multiple potential solutions simultaneously, accelerating the convergence to an optimal or near-optimal solution.

Nevertheless, the computational demands of stochastic optimization are significantly higher, often requiring advanced algorithms and substantial computational resources to manage the complexity of simultaneous supply chain and equipment design optimization (Tolooie et al. 2020). Furthermore, the integration of real-time data and adaptive learning algorithms can enhance the robustness of these models, allowing them to dynamically adjust to changing conditions and new information. This approach can significantly improve the reliability and resilience of supply chain operations, particularly in environments characterized by high volatility and uncertainty. However, implementing such sophisticated models poses additional challenges, including the need for high-quality data, advanced computational infrastructure, and specialized expertise in both supply chain management and advanced optimization techniques (Nzeako et al. 2024). Therefore, while the simplification of equipment design in supply chain models is a common practice to mitigate computational challenges, it underscores the need for ongoing research and development of more robust optimization frameworks that can handle the full complexity of these interdependent systems without compromising on solution quality. This involves not only enhancing the mathematical and algorithmic approaches but also fostering interdisciplinary collaboration to integrate insights from engineering, operations research, computer science, and data analytics. By advancing these integrated frameworks, it is possible to achieve more accurate, efficient, and resilient supply chain designs that fully account for the complexities of both the supply chain and the associated technologies (Belhadi et al. 2022).

Recent advancements in chemical process engineering, spanning design, simulation, and optimization, have significantly enhanced the treatment of supply chains (Gamboa Bernal et al., 2020; Pasha et al. 2021). These advancements have yielded economic, environmental, and social benefits by reducing production and operational costs (Martinez-Lomovskoi et al. 2023), minimizing raw material usage, mitigating environmental emissions (Sanchez–Ramirez et al., 2024), and generating employment opportunities (Baah et al. 2021; Nuñez-Lopez et al., 2018). For instance, Kamalahmadi et al. (2022) examined the minimized economic impact of adding flexibility and redundancy in supply chains, while Hosseini-Motlagh et al. (2020) analyzed economic objectives for a sustainable electricity supply chain network design. On the environmental front, Mohtashami et al. (2020) designed a green supply chain to optimize the reduction of emissions in a transportation fleet's network, and Krishnan et al. (2020) proposed an environmental impact assessment in a food supply chain to improve environmental sustainability. However, during the formulation of all these mathematical models, different simplifications have been made, among them is that during the design and optimization of supply chains, the design of the operating equipment has always remained fixed (Duhbacı et al., 2021; Sansana et al. 2021). This is attributed to the formulation involving a substantial number of equations containing highly nonlinear and nonconvex terms, posing challenges for deterministic optimization methods (Danilova et al. 2022), in conjunction with the difficulty of involving the thermodynamic modeling of this equipment (Jackson and Grossmann, 2001). A few years ago, process units were simplistically treated as black boxes in the design, utilizing deterministic techniques for mathematical model solutions (Li et al. 2024; Subramanian et al. 2021). However, the outcomes deviated considerably from reality, since the design of this equipment is considered fixed, and the simplifications made do not consider the variability of costs that may arise when varying the size of any of the equipment or the energy consumption required by them. This cost has a great impact on the total cost of designing a supply chain (Yeomans and Grossmann, 1999).

Consequently, hybrid strategies have been introduced recently, optimizing process units stochastically and subsequently performing deterministic supply chain optimization (Dhiman, 2021; Iwendi et al. 2021). Although these strategies yield superior results, the sequential execution significantly escalates computational time (Huerta-Rosas et al. 2024; Tinoco–Saenz et al., 2022). Some notable contributions in hybrid optimization include the following. Dong et al. (2023) proposed a novel hybrid robust-interval optimization to facilitate flexible and robust uncertainty planning to reduce operational costs; Resat (2020) presented a novel solution methodology to design sustainable delivery systems in urban areas, and Saini et al. (2021) achieved a multi-objective hybrid machine learning optimization approach for enhanced cell biomass production. On the other hand, in some of these works, different simplifications have been made, to relax the mathematical models addressed and to be able to easily solve the bilinear and non-convex terms that are generated in mathematical programming. Below are some of the contributions that have been made in this regard. Spiegler et al. (2016) provided a systematic methodology for the rigorous analysis and design of nonlinear supply chain dynamics models, especially when overly simplistic linear relationship assumptions are not possible or appropriate. Ponte et al. (2017) showed that in some works nonlinearity is often significant and should not be ignored, and You and Grossmann (2008) treated some objectives as parameters to fix certain values and approximate Pareto's optimal curves. In addition, there are works where it is reported that by using these hybrid optimization strategies it is possible to solve a complex problem. For example, Hernandez-Perez et al. (2020) proposed a hybrid optimization strategy that was applied to scheduling of hydraulic fracturing process to obtain shale gas, Lopez-Flores et al. (2022) presented an approach to interplant heat integration and thermal engines that considers the equitable allocation of resources among different industrial plants and recently Liñan et al. (2024) proposed a hybrid method for the design of a thermal system and a sequence of reactive distillation column were an improved in convergence was obtained.

Despite these advancements, no work has rigorously considered the design of equipment within a supply chain. Therefore, in this work, a general hybrid methodology is proposed for the solution of supply chains, where the deterministic part resolves the distribution of resources, while the rigorous design of the equipment is simultaneously resolved through metaheuristic optimization. This proposed methodology leverages the strengths of both deterministic and stochastic approaches, aiming to address the limitations of current models. By integrating metaheuristic techniques, such as Differential Evolution with a Tabu List (DETL), simulated annealing, or particle swarm optimization, the design process can more accurately reflect real-world complexities. These techniques allow for the exploration of a broader solution space, accommodating nonlinearities and nonconvexities that deterministic methods struggle with.

The novelty and contribution of this work lie in the concurrent optimization of both the supply chain logistics and the detailed design of production equipment. This hybrid approach ensures that the design and operational aspects of the supply chain are optimized concurrently, leading to more coherent and practical solutions. For instance, deterministic optimization can handle the logistical aspects, such as route planning and resource allocation, while metaheuristic optimization can fine-tune the equipment design to enhance efficiency and reduce environmental impact. By addressing the equipment design rigorously and in tandem with supply chain optimization, this methodology provides a more integrated and holistic solution, potentially leading to significant improvements in performance, cost-efficiency, and sustainability. Moreover, this work introduces a level of flexibility and robustness previously unattained in supply chain modeling. In addition, the proposed hybrid methodology can be tailored to various industries and supply chain structures, making it a versatile tool for a wide range of applications. This work represents a significant advancement in the field of supply chain optimization by offering a novel methodology that bridges the gap between supply chain logistics and equipment design. The integration of deterministic and metaheuristic optimization techniques not only enhances the precision and applicability of the models but also sets a new standard for addressing the inherent complexities of supply chain systems. This hybrid approach promises not only to improve operational efficiency and reduce costs but also to enhance the sustainability and resilience of supply chains, making it a critical development for future research and practical applications in the field.

2. Problem Statement

Traditional optimization methods in supply chain management are usually based on deterministic models. However, in the mathematical formulation for solving them, many simplifications are made, which largely affect the total cost of the supply chain design. One of the main simplifications made is to assume the design of process equipment as black boxes, where only one associated cost parameter is assigned per unit of the desired product.

These types of simplifications are usually made because the rigorous design of this equipment requires the use of stochastic methods, which require a high computational time. On the other hand, deterministic models, while accurate, have difficulty adapting to uncertainties such as demand variability, fluctuations in delivery times, and supply disruptions (Chen et al. 2023). Moreover, the global nature of supply chains introduces additional layers of complexity, including multimodal transportation, diverse regulatory environments, and variable cost structures. Additionally, in most reported works, the design parameters of the equipment operating in a supply chain are kept constant (Grossmann et al. 2005) to avoid resolving high nonlinearities and non-convex terms. However, the costs associated with equipment design have a significant impact on the overall solution of a problem, making it a critical point to consider in the general design of a supply chain (Hasani et al. 2021; Hernandez-Perez and Ponce-Ortega, 2021). Therefore, more attention needs to be paid to these factors, which necessitate a more sophisticated optimization approach that can seamlessly integrate different techniques to leverage their respective strengths in a single methodology. As shown in Fig. 1, to solve this problem where both deterministic optimization and stochastic optimization are required, a program is required that functions as an intermediary between the two-programming software used, because the programming language is very different and it is not possible to maintain direct interaction. Therefore, this paper proposes a general method for solving supply chains using a hybrid optimization tool, where the variability of design parameters is considered to be incorporated in the production and distribution of resources. In this way, the distribution of resources is optimized sequentially with the design of the equipment, in case there are any fluctuations in demand, or adjustments required in the process.

3. Methodology

The following general methodology was proposed for the design of equipment and distribution of resources in a supply chain, where a hybrid mathematical algorithm (deterministic and metaheuristic) is presented for process optimization (Fig. 2). The step-by-step methodology (Fig. 3) is listed below:

1. Generation of decision variable values by the metaheuristic optimization algorithm.
2. Creation of values for the uncertainty parameters in a random value generator.
3. Send the values of the decision variables using the linking program.
4. Calculation of objective functions by the deterministic optimization algorithm.
5. Import of objective function values by the linker program.
6. Analysis of the values of the objective functions by the stochastic optimization algorithm.

The flowsheet starts with rigorous equipment design optimization, a synergistic approach using a metaheuristic optimization that uses differential evolution with a tabu list to find solutions in highly non-convex problems. For solving this optimization, Aspen Plus and Visual Basic programming in Excel were employed. Aspen Plus facilitated the exchange of decision variables, while Visual Basic handled iterative interactions with metaheuristic algorithms until achieving the desired objective. Subsequently, the values of the desired variables are extracted as parameters for the rigorous design of the equipment and are used by the deterministic optimization program.

Concurrently, deterministic optimization was conducted using the GAMS (General Algebraic Modeling System) software. This phase aimed to find the optimal solution for a predefined objective function while strictly adhering to specified constraints. By utilizing both Aspen Plus and GAMS, this dual software approach ensured comprehensive optimization of equipment design intricacies and objective fulfillment within the supply chain framework.

In addition to the differential evolution with a tabu list and the deterministic programming, the hybrid optimization strategy relies on a set of routines developed within the same Visual Basic tool. These routines enable the exchange of information between metaheuristic and deterministic optimization algorithms, allowing each to address its respective part of the problem. Additionally, a routine is necessary to incorporate randomness into the problem by generating uncertain values for some parameters in the mathematical model. The key routines in this methodology are as follows:

- Radom values generator: Random values are generated in a Visual Basic routine to serve as parameters that are typically assumed to be constant within the mathematical model.
- Linker program code: This is a collection of subroutines that establish communication between the various platforms involved, facilitating the transfer and retrieval of data used throughout the optimization process.

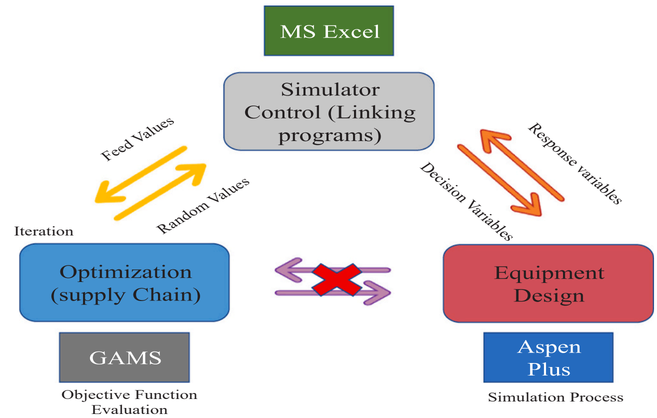

Fig. 1. Problem Statement.

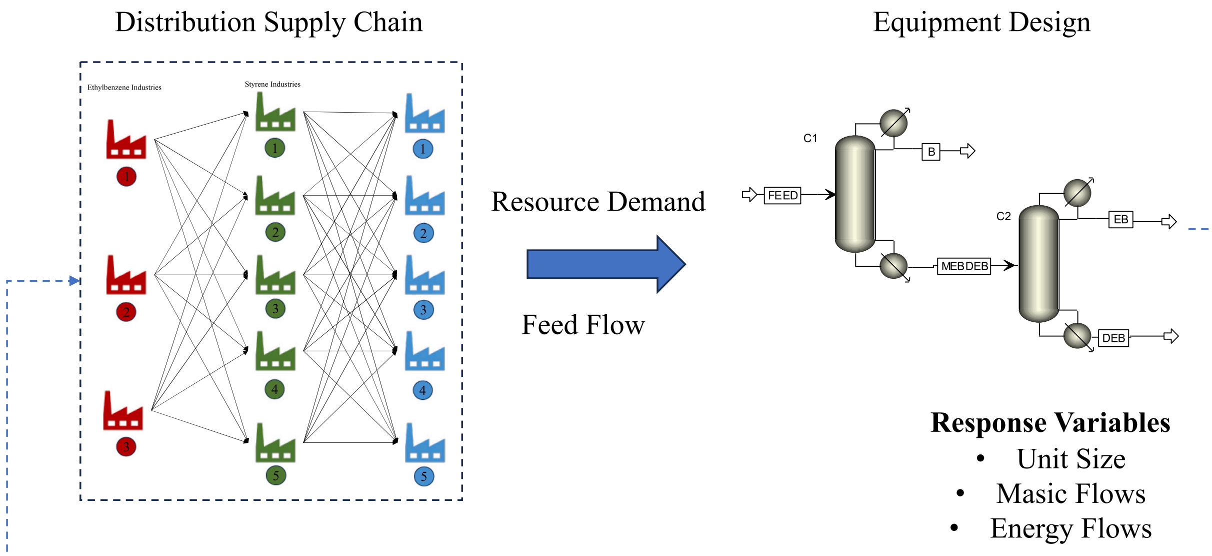

Fig. 2. Proposed methodology for hybrid optimization.

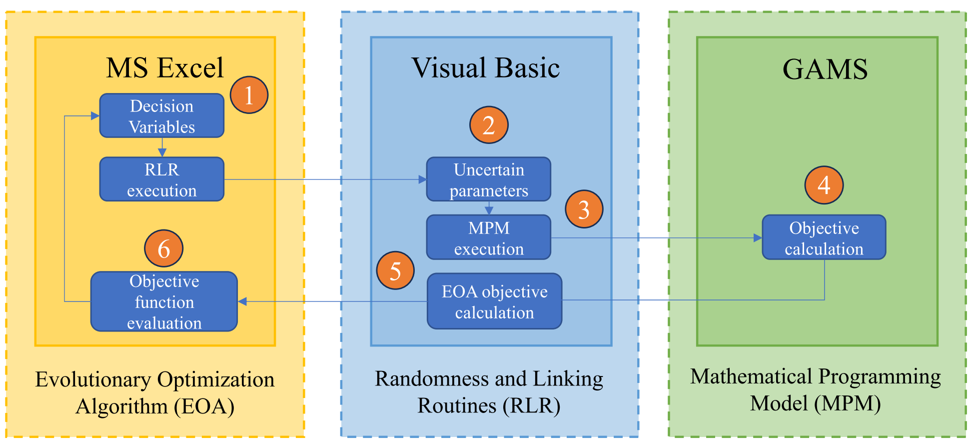

Fig. 3. Step-by-step methodology for hybrid optimization.

4. Case study

In this section, a case study is presented to show the applicability of the proposed methodology. The case study represents a mathematical programming model for a supply chain for the production and distribution of polystyrene in Mexico. However, since it is a general methodology, it can be used to rigorously design any supply chain. It is only necessary to adjust the model of the required equipment in the stochastic programming software, as well as the variables and parameters subject to the distribution of the supply chain to be solved.

In recent years, there has been a large increase in the production of the plastics industry (Pathak et al. 2023). At a global level, in the year 2000, around 150 million tons of this resource were consumed, while in 2023, around 400 million tons of it were used, almost three times as many tons of plastic. In Mexico, plastic production is approximately 3.8 million tons per year; however, in 2022 an apparent consumption of 6 tons was reported, so in order to satisfy the demands of this product, it must be imported from other countries (Angeles-Hurtado et al. 2023). Among the main plastics used in Mexico are polyethylene, polypropylene and polystyrene, applied mainly in the fishing, agricultural, textile and packaging sectors. However, in Mexico there is a greater number of processing plants to produce polyethylene and polypropylene; therefore, a large amount of the polystyrene used in Mexico must be imported. Polystyrene is a thermoplastic derived from the petrochemical industry; its main uses are in the construction industry and the food industry. In Mexico, the production and distribution process of polystyrene face several problems, from the availability of the raw material to produce this compound, to the supply chain for its final distribution throughout the country. In some other countries, studies have been carried out on polystyrene supply chains, focused on the distribution of the product and the mitigation of the emissions generated; however, these studies do not contemplate the simultaneous design of the used equipment during the optimization supply chain (Muthukumar et al. 2024; de Souza Junior et al., 2020).

The proposed methodology was implemented for the design and distribution of a polystyrene production process in México. The 5 most important polystyrene industries in central Mexico were taken into account, which have 5 options in this same region to obtain their raw material, which is styrene, in turn, the styrene industries have 3 plants where the synthesis and separation of ethylbenzene is carried out. Table 1 shows the industries used for the case study as well as the capacity of each of the industries in tons per year and Fig. 4 shows the geographical location of each of them.

The objective was to satisfy the demand for polystyrene in Mexico, which is 600,000 tons per year. To produce 1 kg of polystyrene, 1.032 kg of styrene are required; and to produce 1 kg of styrene, 1.043 kg of ethylbenzene are needed. Therefore, approximately 646,000 tons of ethylbenzene are required per year to produce the amount of

Table 1
Mexican industries used polystyrene production and their production capacities in tons per year.

	Ethylbenzene	Styrene	Polystyrene
1	Special Representations HCR (300,000)	Atlanta Quimica (200,000)	Americas Styrenics (100,000)
2	Avantar Performance Materials (250,000)	Brenntag Mexico (150,000)	Bulkmatic from Mexico (220,000)
3	Mexican Oil (200,000)	Dow Quimica Mexicana (170,000)	Chevron Oil Latin America (180,000)
4		Helm from Mexico (130,000)	Resirene (110,000)
5		Mexican Oil (110,000)	Laplex (80,000)

Fig. 4. Geographical location for considered industries in Mexico.

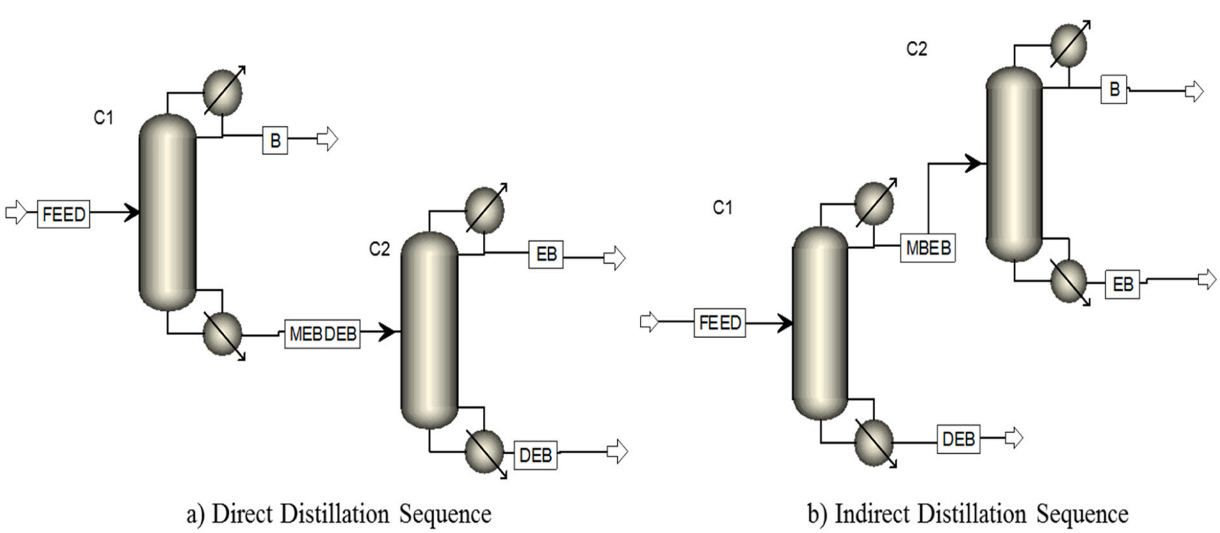

Fig. 5. Considered distillation sequences for separation.

polystyrene required by the country. The base case considered in this work is a simplified plant to produce ethylbenzene from ethylene and benzene. All kinetic and design parameters for this base case were taken from Luyben (2002). In this particular case, the demand for polystyrene to be satisfied is a parameter. Therefore, there is no need to generate random values for the objective functions of the mathematical model in the deterministic part. However, this methodology can be used with different supply chains where the objectives are set in different ways.

4.1. Distillation sequences design

For the separation process, two distillation sequences were selected: a conventional direct sequence (SD) (Fig. 5**a**) and a conventional indirect sequence (SI) (Fig. 5**b**). These sequences were designed using Aspen Plus with the DSTW module, leveraging its capability for rigorous equipment design. The reflux ratios were chosen to be 1.3 times the minimum values required for efficient separation (A value of 1.3 times the minimum reflects a common practice in the design of distillation columns). This increase above the minimum is used to ensure more efficient and robust separation, considering potential variations in operating conditions and component properties. Additionally, the operating pressures were set at 4.5 atm for the first column and 2 atm for the second column (These pressures are designed to optimize the balance between separation efficiency and energy consumption, ensuring that the distillation process operates within economically and environmentally viable parameters). The above parameters were taken as initialization values for the optimization of the separation column design mentioned above (Alpuche-Manrique et al. 2011). In summary, these parameters were selected to optimize the separation efficiency and operational performance of the distillation columns within the specified process constraints. Moreover, these design choices ensure robust separation performance under varying operational conditions and component properties, aligning with industry standards for reliable distillation operations. Therefore, the decision variables considered for the design resolution of this equipment are the stage number, the feed stage, the column reflux, the column diameter, and the distillate flow.

In the indirect sequence, the feed to the first column is a mixture of benzene (B), ethylbenzene (EB) and diethylbenzene (DEB), with a molar composition of 48 %, 46 % and 6 %, respectively. The feed flow is 1738 kmol/h. In the first column, the DEB is separated at the bottoms, while a mixture of benzene and ethylbenzene is fed to a second column in which the EB is recovered at the bottoms of the column with a purity of 0.99. In the direct sequence, there is the same feed flow and the same composition to the first column, however in this sequence, the benzene goes overhead, and a mixture of DEB and EB (bottoms product) is fed to the second column in which ethylbenzene is recovered as a distillate product. The optimization of the separation column parameters was obtained by means of metaheuristic tools, using differential evolution with a tabu list.

4.2. Supply Chain mathematical programming

For the distribution of polystyrene, the superstructure shown in Fig. 6 represents the supply chain for this product. Material balances were carried out for the conversion of ethylbenzene to styrene and subsequently to polystyrene, and the distribution of these resources across the different industries involved. These balances were programmed and solved in the GAMS software with their respective objective functions and restrictions associated with the model. The mathematical model is a linear programming model (LP), which was solved on a computer with a Core i7 processor with a RAM memory of 32 GB. The total computing time for the proposed tool was approximately 22 hours.

The objectives to be solved for this case study are the minimization of the total cost of the process (Eq. 1), which consists of the cost of the distillation equipment plus the cost of processing and distribution of resources in the supply chain; and the minimization of the environmental impact through the evaluation of Eco indicator 99 (Eq. 2). The

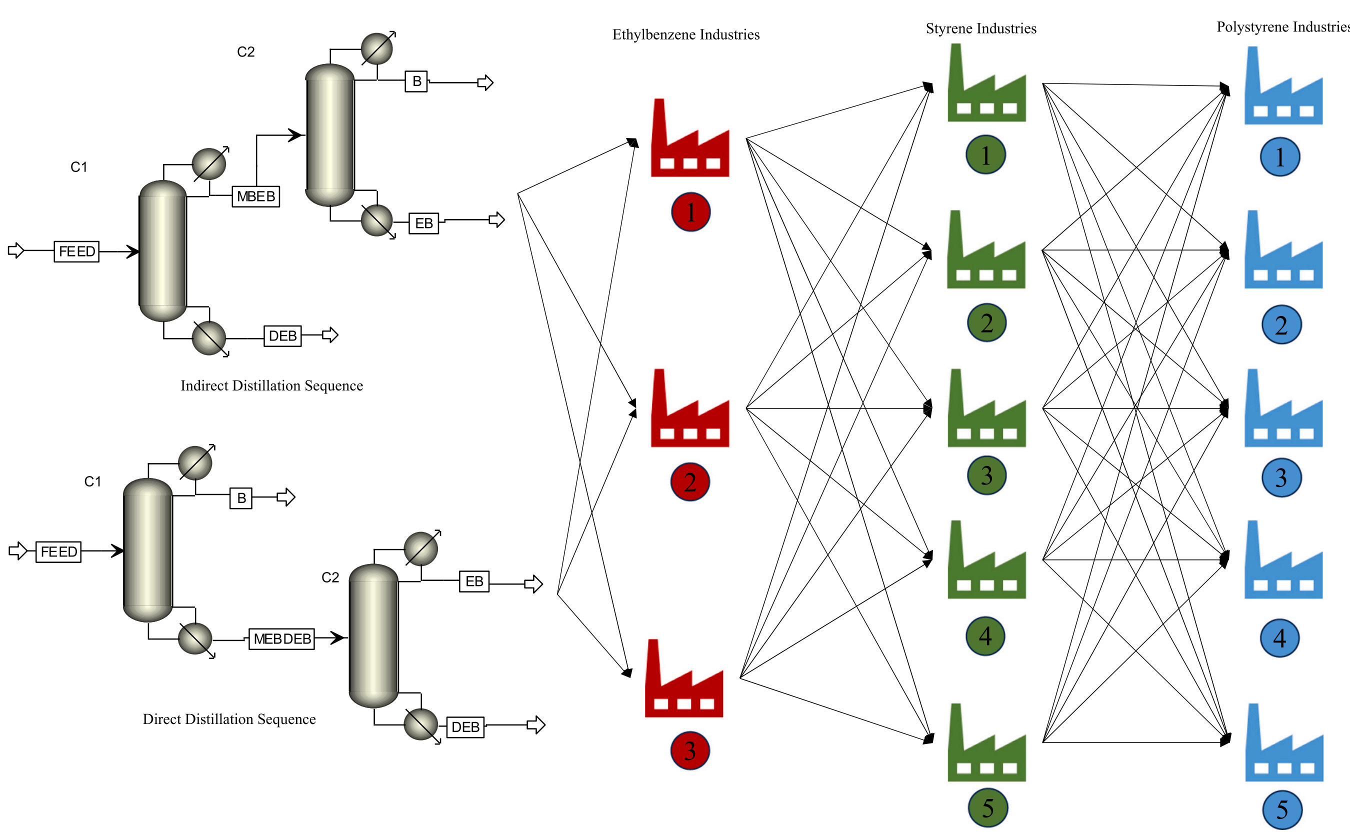

Fig. 6. Superstructure for polystyrene production.

objective functions are listed below:

$$Min\ TotalCost = TotalProdCost + TotalDesignCost \tag{1}$$

$$Min\ EI99 = \sum_{b}\sum_{d}\sum_{k\in K}\delta_d\omega_d\beta_b\alpha_{b,k} \tag{2}$$

where δ_d is the normalization factor for damage in category *d*, ω_d is a weighting factor for damage in category *d*, β_b represents the total amount of chemical *b* released per unit of reference flow due to direct emissions and $\alpha_{b,k}$ is the damage caused by category *k* per unit of chemical *b* released to the environment. Table 2 shows the values used for eco-indicator calculation.

The total cost of the distillation equipment is equal to the operating costs and the investment costs related to this equipment. These are calculated through stochastic tools, using genetic algorithms.

To calculate the cost of styrene production ($PC_{Styrene}$), the sum of the cost factor ($CostSty_S$) associated with each industry by the flow of styrene produced ($ProdSty_S$) in each of those industries was used.

$$PC_{Styrene} = \sum_{S} CostSty_S ProdSty_S \tag{3}$$

While the cost of styrene production ($PC_{Ehylbenzene}$) was calculated through the cost factor ($CostEthyl_E$) associated with each ethylbenzene industry by the flow of ethylbenzene ($ProdEthyl_E$) corresponding to each of these industries.

$$PC_{Ethylbenzene} = \sum_{E} CostEhyl_E ProdEthyl_E \tag{4}$$

To meet the demand for polystyrene the following equations were used:

$$PolystyreneDemand = Polystyrene \tag{5}$$

where *PolystyreneDemand* is a parameter of the quantity of polystyrene that is desired to be produced and *Polystyrene* is the total flow of polystyrene produced by all industries, which must be equal to the required demand.

To produce 1 kg of polystyrene, 1.032 kg ($Factor_{styrene}$) of styrene are required ($ReqSty$).

$$ReqSty = Factor_{styrene} Polystyrene \tag{6}$$

And to produce 1 kg of styrene, 1.046 kg ($Factor_{ethyl}$) of ethylbenzene are required ($ReqEthyl$).

$$ReqEthyl = Factor_{ethyl} ReqSty \tag{7}$$

The total flow of polystyrene, styrene and ethylbenzene used is equal to the sum of the flow from each of the industries where these compounds are produced.

$$Polystyrene = \sum_{P} ProdPoly_P \tag{8}$$

Table 2
Parameter values for eco-indicator 99.

Impact category	Steel (points/kg)	Steam (points/kg)	Electricity (points/kg)
Carcinogenics	6.32E−03	1.18E−04	4.36E−04
Climate change	1.31E−02	1.60E−03	3.61E−06
Ionising radiation	4.51E−04	1.13E−03	8.24E−04
Ozone depletion	4.55E−06	2.10E−06	1.21E−04
Respiratory effects	8.01E−02	7.87E−07	1.35E−06
Acidification	2.71E−03	1.21E−02	2.81E−04
Ecotoxicity	7.45E−02	2.80E−03	1.67E−04
Land occupation	3.73E−03	8.58E−05	4.68E−04
Fossil fuels	5.93E−02	1.25E−02	1.20E−03
Mineral extraction	7.42E−02	8.82E−06	5.70E−06

$$ReqSti = \sum_{S} ProdSty_S \tag{9}$$

$$ReqEthyl = \sum_{E} ProdEthyl_E \tag{10}$$

Taking as a restriction the production capacity of each of these industries, the following equations highlight that the individual flow of each polystyrene, styrene and ethylbenzene industry cannot be greater than the individual production capacity of each of the industries.

$$ProdPoly_P \leq CapPoly_P \quad p\epsilon P \tag{11}$$

$$ProdSty_S \leq CapSty_S \quad s\epsilon S \tag{12}$$

$$ProdEthyl_E \leq CapEthyl_E \quad e\epsilon E \tag{13}$$

5. Results and Discussion

The proposed methodology was implemented for the simultaneous optimization of the equipment design and the supply chain for the production and distribution of polystyrene in Mexico. illustrate the Pareto curve for the direct and indirect distillation sequence optimization, respectively, showcasing all possible optimal solutions. By utilizing Pareto curves, a representative scenario was selected for each distillation sequence (red points in both pareto graphics), striving to balance economic and environmental objectives.

In a nuanced exploration of the comparative analysis of distillation sequences (Table 3), Table 4 meticulously outlines the design parameters, offering a comprehensive perspective on the outcomes resulting from the application of both conventional direct and indirect sequences. Notably, the direct sequence stands out by first separating benzene, the most abundant component, which adds a layer of specificity to the intricate dynamics of the distillation process. While Table 5 shows the parameters used by the Differential Evolution with a Tabu List method.

The subsequent scrutiny of the distribution of polystyrene in Mexico reveals a notable similarity between the two sequences, attributed to the exclusive reliance on ethylbenzene availability, a factor that remains consistent at the conclusion of both separation sequences. As the focus shifts to the economic dimensions, a closer examination of the total cost and Eco-indicator of the system for each distillation sequence unveils the direct separation process as the more economically favorable option (Fig. 7).

Furthermore, the proposed hybrid methodology leverages the strengths of deterministic and metaheuristic optimization techniques. By integrating these approaches, the methodology not only enhances the precision of the equipment design but also improves the overall efficiency and sustainability of the supply chain. The application of metaheuristic techniques enables the exploration of a broader solution space, accommodating nonlinearities and nonconvexities that deterministic methods struggle with. The comprehensive optimization process involves a detailed analysis of various factors influencing the supply chain, including production rates, transportation logistics, and distribution networks. By concurrently optimizing these elements with the equipment design, the methodology ensures a more coherent and practical solution. This integrated approach also considers fluctuations in demand and potential adjustments required in the production process, thereby enhancing the adaptability and resilience of the supply chain.

In addition, the environmental impact assessment forms a crucial part of the optimization process. The Eco-indicator, used to evaluate the environmental performance of each distillation sequence, provides valuable insights into the sustainability of the production and distribution processes.

By prioritizing scenarios that strike a balance between economic and environmental objectives, the proposed methodology supports the development of more sustainable supply chains.

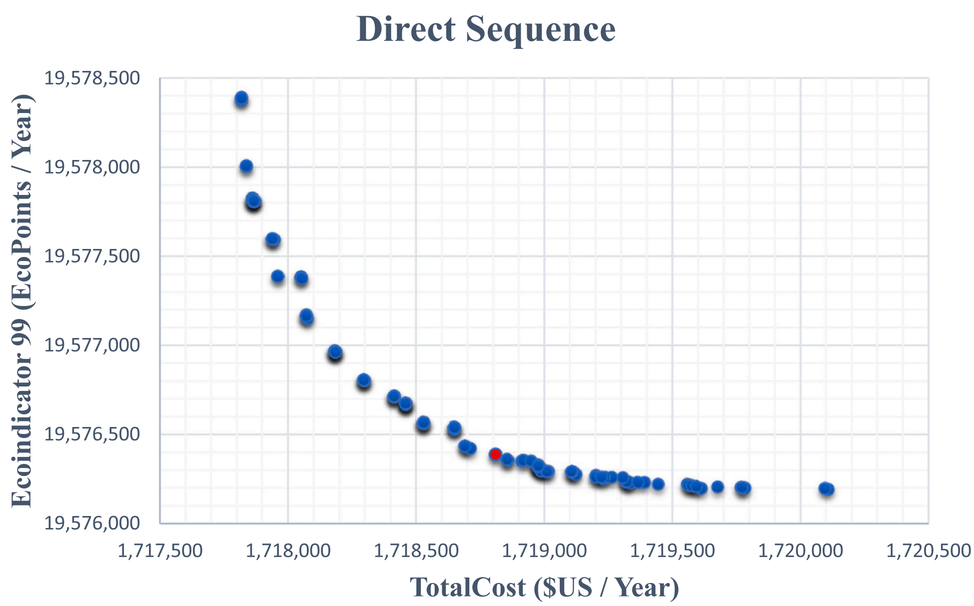

Fig. 7. Optimization for direct distillation sequence.

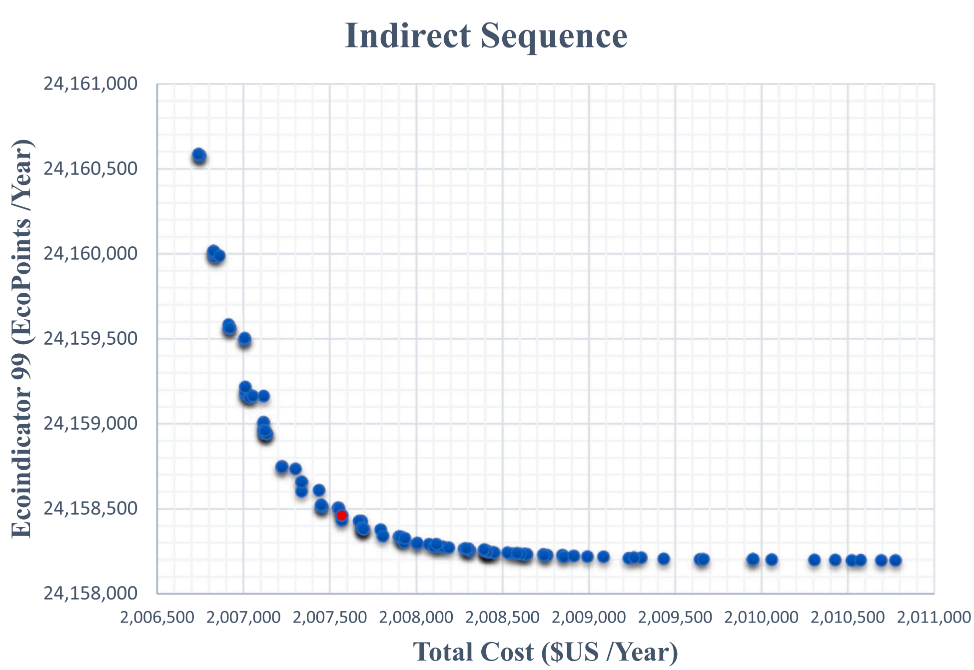

Fig. 8. Optimization for indirect distillation sequence.

Table 3
Range of parameter searching.

Type of variable		Column 1	Column 2
		Search Range	
Number of Stages	Discrete	4–50	3–100
Feed Stage	Discrete	5–49	4–99
Relux Ratio	Continuos	0.1–10	0.2–10
Top Rate (kmol/h)	Continuos	970–1000	690–700
Diameter (meter)	Continuos	0.2–5.0	0.1–5.0

Fig. 9 shows the optimal direct separation sequence, as well as all the flow streams in the columns and the compositions of each of them. It can be observed in the distillate of the second column, that a stream of ethylbenzene (compound of interest for the case study) with a purity of

Table 4
Design parameters for conventional distillation.

	DS	IS
Stages/feed stage of column 1	49/30	30/15
Stages/feed stage of column 2	23/11	10/7
Pressure column 1/column 2 (bar)	4.5/2	4.5/2
Reflux ratio 1/reflux ratio 2	0.60/9.33	0.20/8.85
Feed stream flowrate (kmol/h)	1738	1738
Distillate flowrate 1 (kmol/h)	978	1668
Bottoms flowrate 1 (kmol7h)	760	70
Distillate flowrate 2 (kmol/h)	690	978
Bottoms flowrate 2 (kmol/h)	70	690
Reboiler heat duty (Mcal/h)	21,172	28,789

Table 5
Differential Evolution with a Tabu List parameters.

Parameter	Value
Population size	120
Maximum generations	500
Tabu List	60
Cross Over Probability	0.9
Mutation Probability	0.3
Tabu Radius	0.0001

0.998 is obtained. Fig. 10 shows the flows from the separation columns for the indirect sequence, wherein the first column diethylbenzene is obtained from the bottom; and a mixture of mostly benzene and ethylbenzene as distillate, which enters a second column where the ethylbenzene flow with a purity of 0.997 is obtained from the bottom.

On the other hand, Table 4 shows that most of the variables of interest for the design of the columns, such as the number of stages and the reflux ratio, are higher for the direct distillation sequence than the indirect sequence. However, the reboiler heat duty is higher for the indirect separation case, which indicates that it is a variable that has more weight when calculating the total cost of the equipment design, since the data show a higher total cost for the indirect separation sequence.

This economic advantage is further accentuated by the intricate resource interconnection flows between the ethylbenzene, styrene, and polystyrene industries, meticulously presented in Fig. 11 and . In Fig. 11, it can be observed that there are 646,826 tons of ethylbenzene (688 kmol/h), which corresponds to the demand required by Mexico in recent years. This ethylbenzene can be obtained from both the direct separation sequence and the indirect separation. Subsequently, there are 3 industries where this component is processed. Ethylbenzene Industries 1 and 3 satisfy 300,000 tons and 200,000 tons, respectively, which represents the maximum production capacity of these industries, while Industry 2 processes the remaining 145,826 tons of ethylbenzene needed.

The mathematical programming code chose the industries that would operate at their maximum capacity based on the associated costs of production and transportation.

Table 6 shows the interconnection flows between the ethylbenzene and styrene industries, whereas Table 7 shows the interconnection flows between the styrene and polystyrene industries. Notice that the

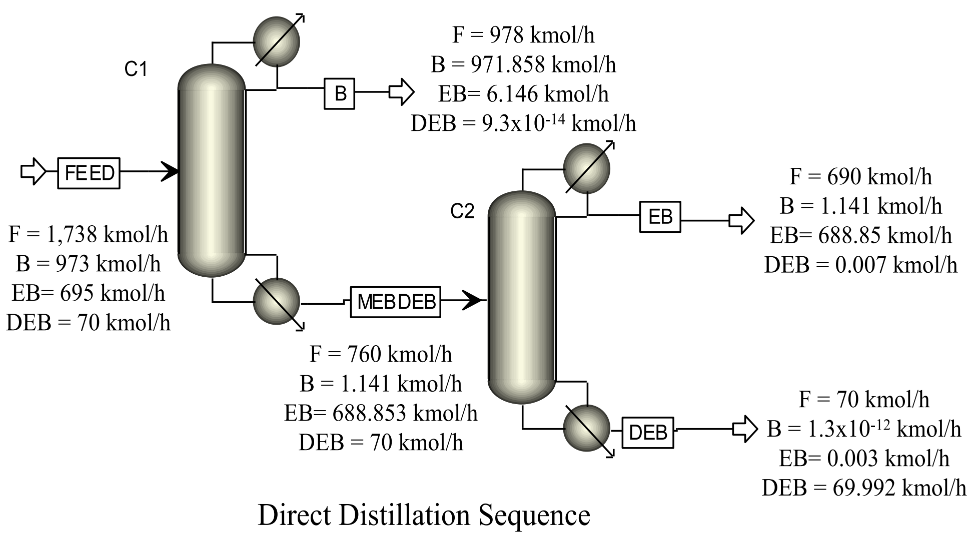

Fig. 9. Optimal solution for direct sequence distillation.

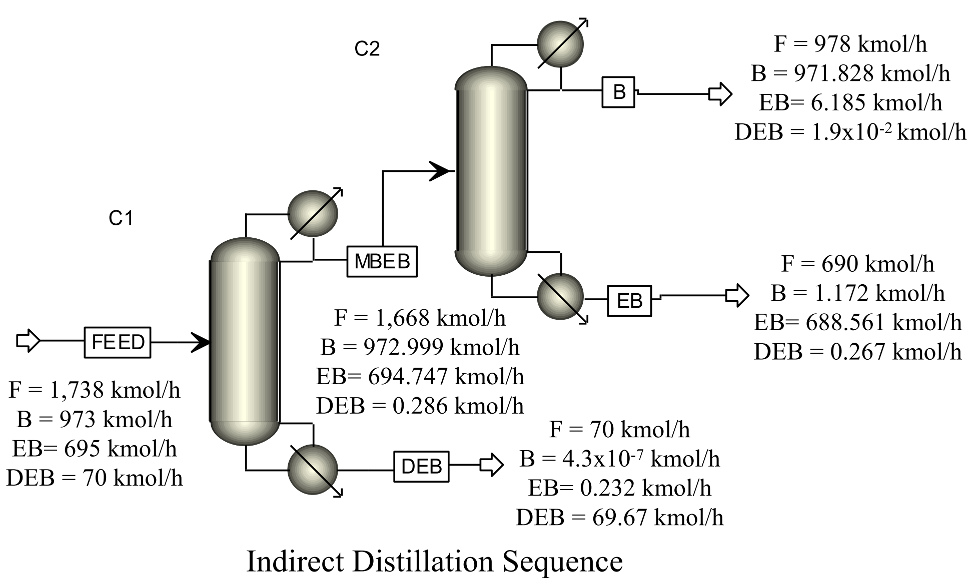

Fig. 10. Optimal solution for indirect sequence distillation.

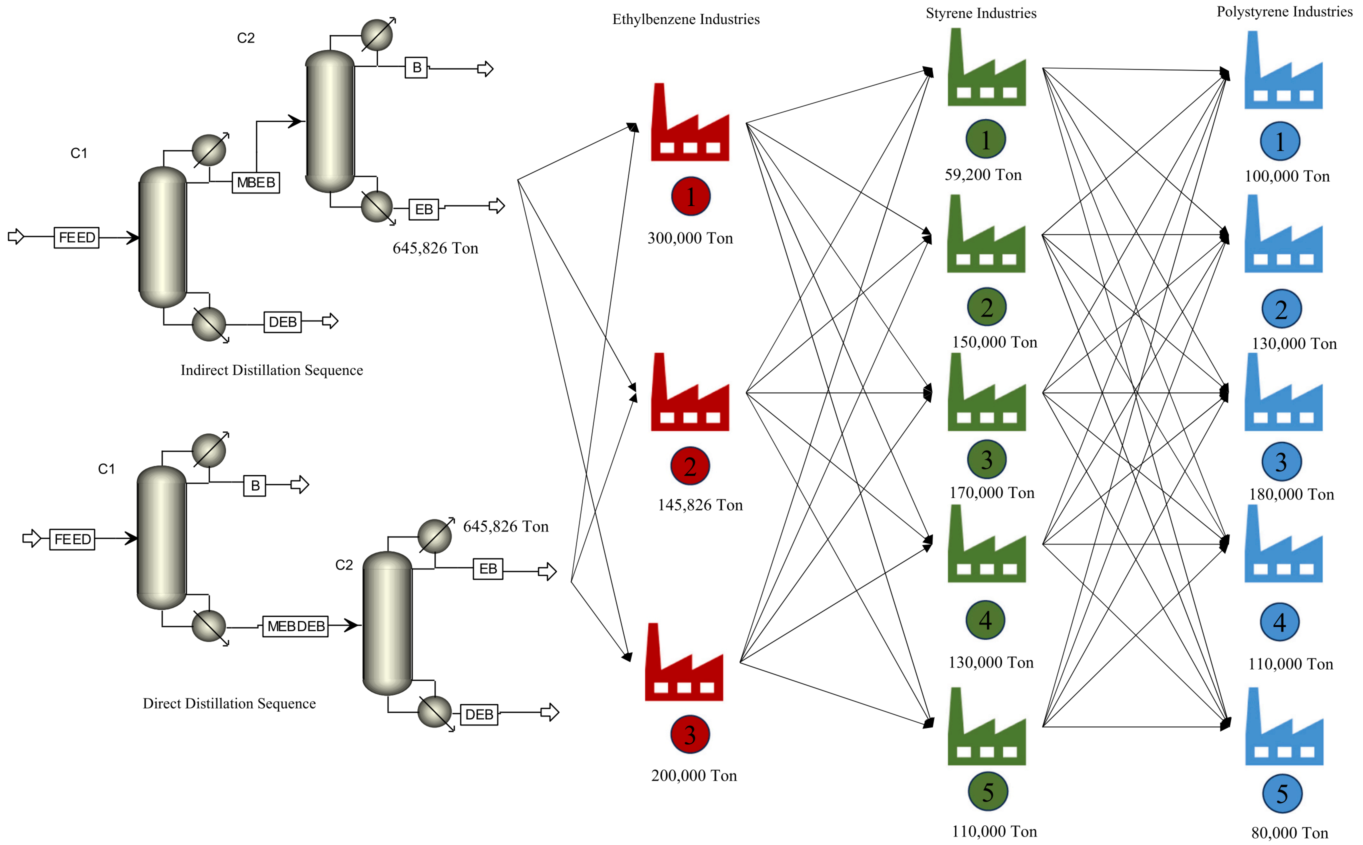

Fig. 11. Production by each of the industries.

Table 6
Tons of ethylbenzene sent to each styrene industry.

		Ethylbenzene		
		1	2	3
Styrene	1	30,000	0	31,746
	2	125,000	31,450	0
	3	130,000	20,000	27,310
	4	0	94,376	41,214
	5	15,000	0	99,730
		300,000	145,826	200,000

Table 7
Tons of styrene sent to each polystyrene industry.

		Styrene				
		1	2	3	4	5
Polystyrene	1	0	20,000	0	39,200	0
	2	35,000	50,000	37,500	0	27,500
	3	50,000	50,000	25,000	20,000	25,000
	4	0	14,160	70,000	35,780	10,060
	5	18,200	0	53,260	18,540	20,000
		103,200	134,160	185,760	113,520	82,560

flow of styrene leaving this ethylbenzene is received by these same industries. This is because 1.043 kg of ethylbenzene is required to produce 1 kg of styrene; the same happens in the polystyrene industries, since 1.032 kg of styrene is required to produce 1 kg of polystyrene.

Likewise, it can be observed that the sum of the polystyrene produced in the 5 industries is 600,000 tons of this compound, which is equivalent to the tons required by the country in recent years to satisfy its needs for this plastic.

Simultaneously, Table 8 provides a comprehensive overview of the optimization objectives for the total cost and environmental impact in both the direct and indirect distillation sequences. Notice that there is a decrease in both objectives in the direct separation sequence compared to the indirect sequence. Specifically, the direct distillation sequence presents a total annual cost that is 6.78 % lower than the indirect separation sequence, as well as 23.40 % less in the value of the Eco indicator, indicating a significant reduction in emissions. According to the data shown in Table 8 and the Pareto curves for the direct and indirect separation sequences, the importance of considering the rigorous design of the equipment becomes evident, as the cost of the equipment represents approximately 40 % of the total cost of the supply chain. The detailed analysis of Table 8 highlights several key insights. Firstly, the direct distillation sequence not only reduces the total annual cost but also significantly lowers the environmental impact, demonstrating its superiority in achieving a balanced optimization between economic and ecological objectives. The substantial reduction in the Eco indicator value underscores the potential for considerable environmental benefits, aligning with contemporary sustainability goals and regulatory requirements.

While both configurations effectively satisfy the demand for polystyrene, the critical distinction lies in the energy supplied, contingent upon the chosen separation method. Consequently, the production cost associated with meeting resource demand in each sequence exhibits noteworthy variations, significantly influencing the economic objective within the overarching solution.

This divergence is expected to persist and gain complexity with the

Table 8
Values for objectives functions.

Objective function	DS	IS
TAC ($US/ Year)	4255,810	4544,570
EI99 (EcoPoints / Year)	19,576,387	24,158,433

inclusion of additional objectives, such as security indicators or social aspects, further underscoring the nuanced impact of the separation approach on the holistic solution and emphasizing the multifaceted nature of the decision-making process in this intricate system.

Furthermore, the direct distillation sequence's ability to reduce emissions significantly positions it as a more sustainable option, crucial for industries aiming to minimize their carbon footprint. This reduction in emissions is particularly relevant in the context of increasing global emphasis on environmental responsibility and sustainability. By choosing the direct sequence, companies can better align with environmental standards and enhance their corporate social responsibility profiles. Additionally, the implementation of the direct distillation sequence offers operational advantages beyond cost and environmental impact. The reduced complexity in the equipment design and operation can lead to lower maintenance requirements and increased reliability, thereby enhancing overall process efficiency. These operational benefits contribute to the long-term viability and competitiveness of the production process.

The strategic selection of distillation sequences, as evidenced by the comprehensive analysis in Table 8, highlights the pivotal role of equipment design in optimizing supply chain performance. The inclusion of detailed equipment design parameters not only influences the immediate economic and environmental outcomes but also affects the long-term strategic decisions related to capacity expansion, technological upgrades, and sustainability initiatives. Moreover, the comparative analysis of the two sequences underscores the necessity of adopting a holistic optimization approach. By integrating both economic and environmental objectives, the proposed methodology ensures that supply chain decisions are robust, resilient, and adaptable to changing market conditions and regulatory landscapes. This holistic perspective is essential for addressing the complex interdependencies within supply chains and for achieving sustainable competitive advantages.

The data presented in Table 8, along with the Pareto curves for the direct and indirect separation sequences, illustrate the significant benefits of considering rigorous equipment design in supply chain optimization. The direct distillation sequence emerges as a superior choice, offering lower costs and reduced environmental impact, while also enhancing operational efficiency and sustainability. This analysis reinforces the importance of a comprehensive and integrated approach to supply chain optimization, where multiple objectives are simultaneously addressed to achieve optimal performance and sustainability in complex industrial systems.

The main importance when considering this type of combined tools is to consider the possible variations that occur in the demand of a supply chain. Because in some works the costs associated with the equipment required by a supply chain are taken as parameters. When increasing or decreasing the demand for a resource, the associated cost of the equipment is usually modified through some mathematical relationship due to the high computing time required to make these models. However, this cost has a great impact when considering the total cost of the process, which is why it is extremely important to consider the rigorous design of this equipment and through these methodologies, these adjustments can be made in less time. Just as the rigorous design of the equipment has a great direct impact on the total cost of the process, so does the environmental impact associated with the process. In this case, for the calculation of the eco-indicator 99, the greatest impact is on the separation of the components of the process flow, due to the large amount required in the reboiler of the separation columns.

6. Conclusions

This study presents a comprehensive approach to exploit the advantages of stochastic and deterministic optimization methods in chemical process engineering for the design of supply chains and process units. The hybrid integration of these methods aims to effectively mitigate their respective limitations. The proposed methodology, illustrated through a detailed case study, showcases the precision of modeling resource distribution in supply chains using deterministic tools, ensuring accurate allocation and transportation of resources. Including rigorous equipment design has a great impact on the final solution of supply chain development, since through the results it can be observed that the largest part of the final solution to the objectives is numerically provided by this process equipment.

Concurrently, the rigorous design of equipment for resource generation is achieved through the incorporation of metaheuristic strategies known for their proficiency in navigating complex, high-dimensional search spaces. This enhances the design process by providing innovative and efficient solutions that may be overlooked by traditional methods.

This integrated methodology not only enhances result reliability but also addresses computational challenges intrinsic to sequential optimization approaches. The framework serves as a robust tool for simultaneous stochastic optimization of process units and deterministic optimization of supply chains. Furthermore, this hybrid strategy emerges as a promising approach for achieving more precise and efficient solutions in complex chemical process engineering scenarios. It provides engineers and researchers with a robust platform to optimize process units and supply chains concurrently, ensuring solutions are theoretically sound and practically feasible. The results show that the direct separation sequence is better both economically and environmentally than the indirect separation sequence; this is because the indirect sequence requires a greater amount of energy in the reboiler to achieve the required separation, which directly impacts on a higher cost and a greater impact on the environment. This integrated approach represents a significant advancement in the field, paving the way for more sophisticated and effective optimization techniques in chemical process engineering.

CRediT authorship contribution statement

Jesus Manuel Nuñez Lopez: Writing – original draft, Software, Methodology, Investigation, Conceptualization. **Eduardo Sánchez-Ramírez:** Writing – review & editing, Validation, Supervision, Software, Investigation. **Juan Gabriel Segovia-Hernández:** Writing – review & editing, Validation, Supervision, Conceptualization. **José María Ponce-Ortega:** Writing – review & editing, Validation, Supervision.

Declaration of Competing Interest

The co authors, Juan-Gabriel Segovia-Hernandez and Eduardo Sánchez-Ramírez are editors for the journal Chemical Engineering Research and Design, but has had no access to, or involvement in, the peer review process for this paper or its handling by the journal at any point

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