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Optimal design of a solar-grade silicon refinery incorporating a fairness approach

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ABSTRACT

The present work aims to obtain an optimal design of a multi-product solar grade silicon refinery under a systematic approach, considering different equity schemes and always seeking to maximize the profit of the facility. The proposed refinery is intensified to satisfy the demands with the use of minimum resources. Our motivation is to include a fairness approach in the design and optimization process which will help to diversify production at a lower cost and with a larger profit. Evaluation under equity approaches of intensified schemes is needed to identify how convenient it is to retain conventional schemes compared to intensified ones. Products of interest to be evaluated include solar grade silicon, tetraethoxysilane at various purities (98.5%, 99.0% and 99.5% mol), silane, dichlorosilane, and monochlorosilane. The optimal profit allocation among these products is analyzed by evaluating different equity schemes (Social Welfare, Rawlsian Welfare and Nash approaches). Results show different income allocations under the equity schemes. These allocations are compared to the optimal design without equity schemes. Results show that the Nash scheme can provide fair trade-offs between the products (such as TEOS, SiH_4, SiH_2Cl_2 and SiH_3Cl) demanded by the market and the refinery's profit.

1. Introduction

Allocating resources (economic, natural or others) among different stakeholders is a common problem in engineering applications. In the optimal design of any multi-product industrial plant, profit is a common measure to determine the allocation of the products of interest. Starting from profit maximization and market demand, an industrial plant and each of its component parts (unit processes) can be designed. This allocation model is commonly known as the classical utilitarian approach (Renouard, 2011).

The utilitarian approach, also called the Social Welfare (SW) approach, may be intuitive. However, on numerous occasions, it can lead to unfair production allocations since the solution may be non-unique. The lack of fairness, or equity, may result from inherent degeneracies in the solution of the model and/or from the approach sensitivity itself (Sampat and Zavala, 2019). Munguía-López and Ponce-Ortega (2021) presented the analysis of different fairness schemes for the allocation of COVID-19 vaccines, and it was observed how the complexity of the allocation increased with the availability of vaccines. This may favor certain sectors of the

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Nomenclature

$/kg	US Dollars per kilogram
$S_{byproducts}$	Sales of the byproducts
$S_{polycrystalline\ silicon}$	Sales of the main product
b	Unit cost of each raw material
c	Cost of each utility E
C1	Column 1
C2	Column 2
Col RD	Reactive distillation Column
DFR	Distillate to feed ratio
E	Utility
FR	Feed Ratio
Hy	Hydrochlorination Reactor
kg/h	kilogram per hour
M$/y	Millions of dollars per year
N	Nash
N/A	Not apply
NLP	Nonlinear programming
P	Pressure
RW	Rawlsian Welfare
RM	Raw material
RR	Reflux Ratio
SiH_2Cl_2	Dichlorosilane
SiH_3Cl	Monochlorosilane
SiH_4	Silane
Si_{SG}	Solar grade silicon
SW	Social Welfare
T	Temperature
T_{Ca}	Thermal Carboreduction;
TEOS	Tetraethoxysilane
RDC	Reactive Distillation Columns

population, for example, the elderly population, but it may also cause disadvantage towards others, becoming a critical case when resources are scarce.

It is evident that the resource allocation among different sectors, parties, or products of interest is a relevant problem in the decision making. Sampat and Zavala (2019) showed a variety of mathematical allocation approaches, as well as the advantages and disadvantages in their application, therefore, it is important not to evaluate with a single scheme, but to study it with multiple schemes and analyze which one is the most appropriate. Usually, resource allocation is carried out using a SW approach. Consequently, obtaining multiple allocations often leads to unfair solutions. Apart from the fact that this approach tends to inadequately capture the scales of the sectors in question. Other alternative approaches have also been proposed to allocate resources. One of those approaches is the Rawlsian Welfare approach (RW), created by Rawls (1971) to address justice. In this scheme, the aim is to maximize the smallest utility, which takes into consideration small stakeholders. However, the scales or sizes of the stakeholders are not captured properly, as it ignores large stakeholders. In an industrial plant, this would mean providing more manufacturing to lower value-added products although this scheme usually identifies non-unique solutions. On the contrary, the Nash approach (N) establishes that the allocation of resources is estimated by maximizing the product of the stakeholders' utilities (Nash, 2016). This function is equivalent to maximizing the sum of the logarithms of the stakeholders' utilities. Through this formulation, it is possible to find unique solutions and capture the scales of the stakeholders. So far, these approaches have not been applied to the design of multi-product plants.

In this paper, the fairness approach has been used in the manufacturing allocation of various products in a solar grade silicon refinery. Ramírez-Márquez et al. (2020) were the first to present a solar grade silicon refinery. They started by generating a process that can take advantage of remaining products to generate high value-added products, resembling the process in a petroleum refinery or a biorefinery. In the work of Ramírez-Márquez et al. (2020), the conceptual design of the refinery is shown to evaluate if it has the capacity to manufacture a portfolio of high value-added products. The results showed that the refinery does have the capacity to reduce the cost of solar grade silicon, with the help of sales of other high market value products. However, there is a tendency for the refinery to opt for maximum production of solar grade silicon and neglect the demand for some of the high value-added products. Therefore, it is necessary to consider the design and optimization of the refinery to meet the demand for each of the high value-added products. This, of course, ensuring the maximum benefit from the multi-product refinery. The present work seeks to diversify the refinery's production in an equitable manner. By means of the mathematical model of the multi-product solar grade silicon refinery, we aim to design the facility taking into consideration the various fairness approaches under the plant utility maximization.

This refinery per se is an intensified process since it takes production units from industrially established processes such as Siemens and Union Carbide. There are currently two industrial processes used in the production of solar grade silicon. The first process is the Siemens process which was developed and successfully utilized in the late 1950′s. It is still, nonetheless, the most widely used process to produce high purity silicon (Payo, 2009). The second process is the Union Carbide process, which thrived in the 1970′s and is also referred to as the monosilicon process (Erickson and Wagner, 1952). These two processes are the basis for the present multi-product solar silicon refinery. The refinery model combines the Siemens and Union Carbide processes to take full advantage of the benefits of both. This process could alone be called an intensified process. In addition, this process incorporates intensified equipment, such as Reactive Distillation Columns (RDC), to produce tetraethoxysilane (TEOS) and a series of high value-added chlorosilanes (silane, dichlorosilane, and monochlorosilane). The RDC is an intensified equipment that links the reactor to the conventional distillation column, and its purpose is to improve chemical conversion. In this process, only the products are removed from the reactive zone while the reactants remain within the reactive zone for further reaction. The importance of implementing reactive distillation columns in the multi-product solar grade silicon refinery is to bypass all material recycling and consequently reduce energy and equipment costs (Sánchez-Ramírez et al., 2018). This is in accordance with the definition of Lutze et al. (2013), where Process Intensification (PI) is defined as the improvement of a process at the operational, functional, and/or phenomena level that can be obtained through the integration of unit operations, the integration of functions and phenomena, or the selective improvement of phenomena for a set of target operations.

It is important to note that the main process units involved in solar grade silicon and other high value-added products refinement were modeled based on experimental information and industrial data. The importance of having in a single multi-product solar grade silicon refinery (the production of all high value-added products) is to meet the demand of each of the markets. In the case of solar grade silicon, the production of solar panels is presented, which in 2018 reached more than 90% of the photovoltaic production (Mints, 2018). And although it might be evident that solar grade silicon for the manufacture of solar cells is the product to be promoted in the plant, it is not always the one that represents the highest net benefit, or the one that the market demands. Products such as TEOS at different purities are attractive to the market since most of their conventional uses include the manufacture of chemical resistant coatings, heat resistant coatings, silicon organic solvents, refractory cement, ceramics, precision casting adhesives, and as binders for the preservation of historical monuments (Mammeri et al., 2006; Duan et al., 2015; Suslick, 1998; Wheeler, 2005). Other uses of these high value-added products include silane (SiH_4) which is relevant in the amorphous solar cell industry (Doyle et al., 1988), dichlorosilane (SiH_2Cl_2) which is a starting material for semiconductor silicon layers found in microelectronics (Fraga et al., 2012) and monochlorosilane (SiH_3Cl) which is used as raw material in the microelectronics industry (Ramírez-Márquez et al., 2016). All these products are in high demand in the microelectronics market (Duan et al., 2015). Therefore, the optimal design of the refinery seeking fair production allocations is imperative to satisfy both profit maximization and market demand.

In this paper, we propose a mathematical modeling approach to find optimal allocations that can be considered fair, according to a set of fundamental axioms. We focus on the study of multiple product allocations of an intensified solar grade silicon refinery. Through the proposed refinery model, several allocations can be identified. The novelty of the present work lies in the fact that the concept of fairness approach has not been applied to any multi-product industry of any kind, even less so in the design stage to guarantee an optimum in the plant's profit. In addition, alternatives for making decisions about the allocations are highlighted. This formulation provides a good approximation to the allocation strategy of manufacturing multiple products for the moment the market demands them and always maximizing the profit of the refinery. In our work, the allocation under various schemes (SW, N, and RW approaches) for the manufacture of various products of the refinery was considered. And, unlike other optimization approaches that seek to maximize or minimize a specific function subject to certain constraints to find compromised solutions, we propose the use of allocation schemes to identify solutions. The objective of using fairness schemes is to make the different production of compounds more equitable. These schemes allow us to identify several solutions to select the most appropriate one.

Everyday profit allocations in any industry are determined by total utility (the sum of the individual utilities). Such an allocation model, known as the classical utilitarian model, is intuitive but can lead to inequitable allocations. This inequality is the consequence of the inherent degeneracies of the solution. In other words, there may be multiple allocations that manage to produce the same total utility. Also, there is an extreme sensitivity of this approach to subsystem scales. Therefore, the problem of utility allocation, production allocation, or any other scenario can be considered as a bargaining game between stakeholders. Schemes such as N and RW provide an axiomatic approach to obtain fair solutions to the multi-product industry design problem.

Table 1 – Prices of raw materials and utilities.

Raw Material	Price [$/kg]
C	59.43 [USD/ton] (U.S. Energy Information Administration, 2021)
SiO_2	60.65 [USD/ton] (American Elements, 2021)
$SiCl_4$	0.75 [USD/kg] (Focus Technology Co., 2021)
C_2H_5OH	0.97 [USD/kg] (Alibaba, 2021)
N_2	47.98 [USD/kg] (The Physics Factbook, 2021)
H_2	4.98 [USD/kg] (NREL Transforming Energy, 2021)
Utilities	Price
Electricity	0.07 [USD/kwh] (Global Petrol Prices, 2021)
Water	0.33 [USD/m^3] (Intratec Solutions, 2021)
Vapor	0.02 [USD/kg] (TLV, 2021)

2. Problem statement

The problem addressed in this paper is as follows. Seven different types of high value-added compounds can be produced in the refinery: solar grade silicon, TEOS 98.5 purity, TEOS 99.0% purity, TEOS 99.5% purity, silane, dichlorosilane, and monochlorosilane. These compounds are defined as interested parties in that they compete for the allocation of the final profit of the refinery. In the following sections, we will visualize the variables related to the design of the multi-product refinery, i.e., which streams are favored in the manufacture of the various products in different equipment, types of feedstocks required for production, external utilities, and operating constraints. The values of raw material and utility costs were addressed with actual market data, as can be seen in Table 1 (Prices are expressed in U.S. dollars).

For the expected product selling prices, the market selling prices were obtained, as shown in Table 2. Each of the selling prices reflected in Table 2 is taken from the real market and it considers an objective scenario in the production of each one of them (PVinsights, 2021; Alibaba, 2021; Alibaba, 2021; Alibaba, 2021; Focus Technology Co, 2021; American Elements, 2021; Zibo Hangyu Import&Export Co., 2021). In the case of polycrystalline silicon price, the selling price of silicon with 6 N purity is considered. It should be noticed that the production cost depends on the considered process as well as the optimized operating conditions. The aim is to find the optimal allocations for the stakeholders, considering both the concepts of equity and economy (profit).

This work presents an optimization approach for the optimal allocation of profit among the generated products in silicon refinery using equity schemes, in particular, each product that comes from different equipment or is under different operating conditions. In this regard, the pursuit to find allocations such as the SW, N, and RW approaches by evaluating equity schemes is proposed. The schematic representation of the system is shown in Fig. 1. Fig. 1 shows how different production routes can be taken within the multiproduct silicon refinery if the process is started with raw materials such as silicon dioxide and carbon. In Fig. 1, it is noticeable that the optimization could opt to produce only one of the products, thus guaranteeing a high profit. An example of this could be done by following the trichlorosilane ($SiCl_3H$) route which would only produce solar grade silicon

Table 2 – Price of each Product.

Polycrystalline Silicon [USD/kg]	6.86 (PVinsights, 2021)
TEOS 99.5 [USD/kg]	3.75 (Alibaba, 2021)
TEOS 99.0 [USD/kg]	2.50 (Alibaba, 2021)
TEOS 98.5 [USD/kg]	1.50 (Alibaba, 2021)
SiH_4 [USD/kg]	88.44 (Focus Technology Co, 2021)
SiH_2Cl_2 [USD/kg]	3.67 (American Elements, 2021)
SiH_3Cl [USD/kg]	3.0 (Zibo Hangyu Import&Export Co., 2021)

(Si_{SG}). However, the market could request the demand for the other products to diversify production towards TEOS at different purities or chlorosilanes (SiH_4, SiH_3Cl or SiH_2Cl_2). Therefore, a fair distribution of the products, which guarantees a design with maximum profit, is necessary for this type of multi-product industry.

The solution to the problem involves the economic objective function of profit, given by the equity schemes since each of the product stakeholders will try to maximize the profit of the refinery. However, an important part to evaluate is whether the nature of the intensified equipment helps in this endeavor by increasing the production of any of the high value-added products. The operating expenses are so high that no profit is generated, or else, the greatest amount of profit is obtained. It is important to note that, in addition to the evaluations under the fairness approach, the refinery was evaluated without any fairness approach to compare results. An important statement is that the ultimate objective of a fairness approach is to shape an allocation distribution in a desirable way. That is, unlike adding demand constraints for each product, the fairness approach establishes fundamental connections that can help guide the selection of appropriate measures to allocate utility in complex decision-making environments.

Four different scenarios are shown. The first one with a refinery operating cost constraint of M$20 per year, the second one with a refinery operating cost constraint of M$15 per year, and the last two scenarios under the uncertainty of the solar grade silicon market price (i.e., 10% above and 10% below of the actual cost). The scenarios were chosen to observe the effect on the design of the multi-product solar silicon refinery, and in turn on the choice of product manufacturing by each equity approach. The first two scenarios will help to study the effect of operating costs by placing the constraints. The other two scenarios aim to analyze the effect of fluctuating product prices to perceive how this alters the design and results of each fairness approach. Lastly, the profit allocations for each refinery design obtained were compared. The fairness of each allocation that may benefit the interested market was analyzed.

The multi-product refinery is shown below. In the Supplementary material section, the material balances can be observed. The optimization of the subrogated model can choose the appropriate feedstock feed flows, the product to be produced, as well as the composition of each product.

2.1. *Case study*

The design of the multi-product solar grade silicon refinery is estimated with a production capacity similar to that of current polycrystalline silicon producing companies, such as Wacker Co. SiO_2 and C feed is considered to cover an average production capacity of 15,000 tons per year of solar grade silicon. Rubber and Plastics News Report (2016). The amount of solar grade silicon may vary depending on the choice of the final products. The modeling of the multi-product solar grade silicon refinery is an extension of the one proposed by Ramírez-Márquez et al. (2020). In the Supplementary material section, the subrogated models of each of the refinery sections are presented. The multi-product solar grade silicon refinery is the result of a strategic combination of Siemens and Union Carbide process steps and the use of a pair of reactive distillation columns to produce high value-added products, such as: TEOS 98.5, TEOS 99.0, TEOS 99.5, silane, dichlorosilane and monochlorosilane.

The multi-product solar grade silicon refinery in general consists of six stages, which are described as follows:

1st stage: In the first stage the production of Si_{MG} takes place. The process is carried out through the carbothermal reduction of quartz with carbon. Here, an electric arc furnace is used, and the temperature is the operating condition to be varied (> 2500 °C). Once Si_{MG} is obtained, it leaves the reactor as a liquid at the bottom of the furnace, allowing it to be introduced into a crucible. Once in the crucible, an oxidative process takes place, which allows it to be separated from many of the impurities, reaching a purity of 99%. The Si_{MG} is poured into ingot molds and cooled for solidification. A temperature of 298 K must be reached in the Si_{MG} through water showers. It is then milled and passed on to the second stage (Ceccaroli and Lohne, 2003).

2nd stage: This is the chlorosilane synthesis reactor stage. In this stage, silicon tetrachloride ($SiCl_4$) is hydrogenated in the presence of Si_{MG}. The remaining impurities such as B, Al, and Fe react and form halides such as BCl_3, $AlCl_3$ and $FeCl_3$. The operating temperatures of this reactor range from 673 to 873 K. Once the reaction has been carried out, a series of chlorosilanes is obtained, such as the remaining trichlorosilane ($SiHCl_3$), dichlorosilane (SiH_2Cl_2) and tetrachlorosilane ($SiCl_4$), in addition to HCl and H_2. These pass through a condensation stage and HCl and H_2 are separated (Ramírez-Márquez et al., 2020).

3rd stage: In this stage, the separation of the chlorosilanes ($SiHCl_3$, SiH_2Cl_2 and $SiCl_4$) is sought. For this stage to happen a train of two distillation columns is generated. In the first column, $SiCl_4$ (being the heaviest) is separated at the bottom. In the second column, a stream of high purity SiH_2Cl_2 is generated through the dome, and high purity $SiHCl_3$ is generated through the bottom.

4th stage: This stage makes use of the high purity $SiCl_4$ stream. The stream is fed to a reactive distillation column to produce TEOS at various purities.

5th stage: In this stage, once a considerable amount of high purity $SiHCl_3$ is produced, it is split into two parts. One part is used to feed the Siemens deposition rector, and

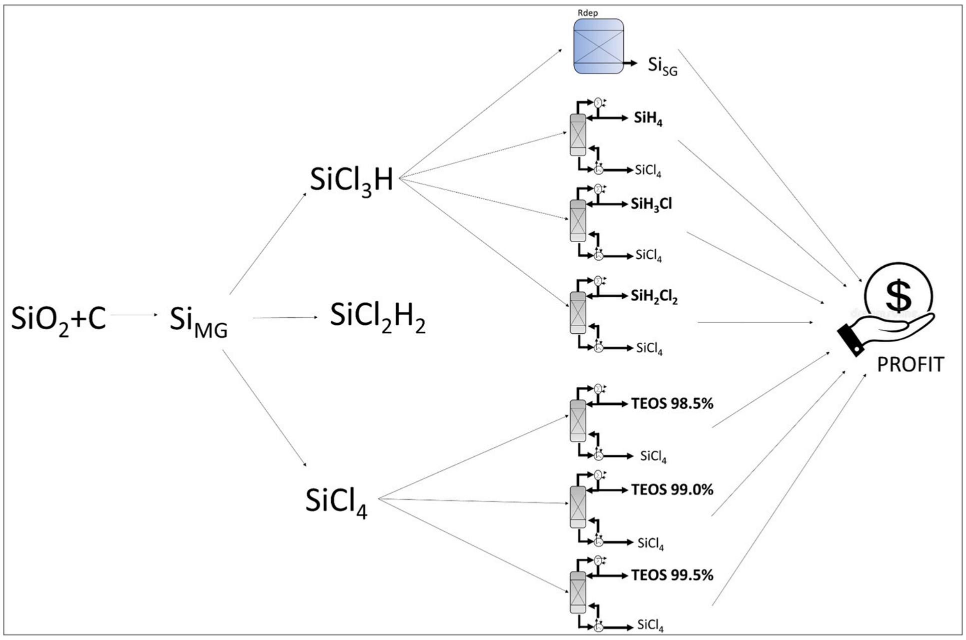

Fig. 1 – General structure of the multi-product solar grade silicon refinery.

another part, left to be decided by optimization, will go to a reactive distillation column, for disproportionation of $SiHCl_3$ to silane (SiH_4), SiH_2Cl_2 and monochlorosilane (SiH_3Cl).

6th stage: The amount of high purity $SiHCl_3$ feeding the Siemens deposition reactor will produce high purity silicon rods. This is accomplished by the thermal decomposition of the trichlorosilane in a hydrogen atmosphere at temperatures of 373–873 K (Del Coso et al., 2008).

Fig. 2 shows the process diagram of the solar grade silicon refinement process and other value-added products used in this work, as well as the entire process sequence and the products generated at each stage.

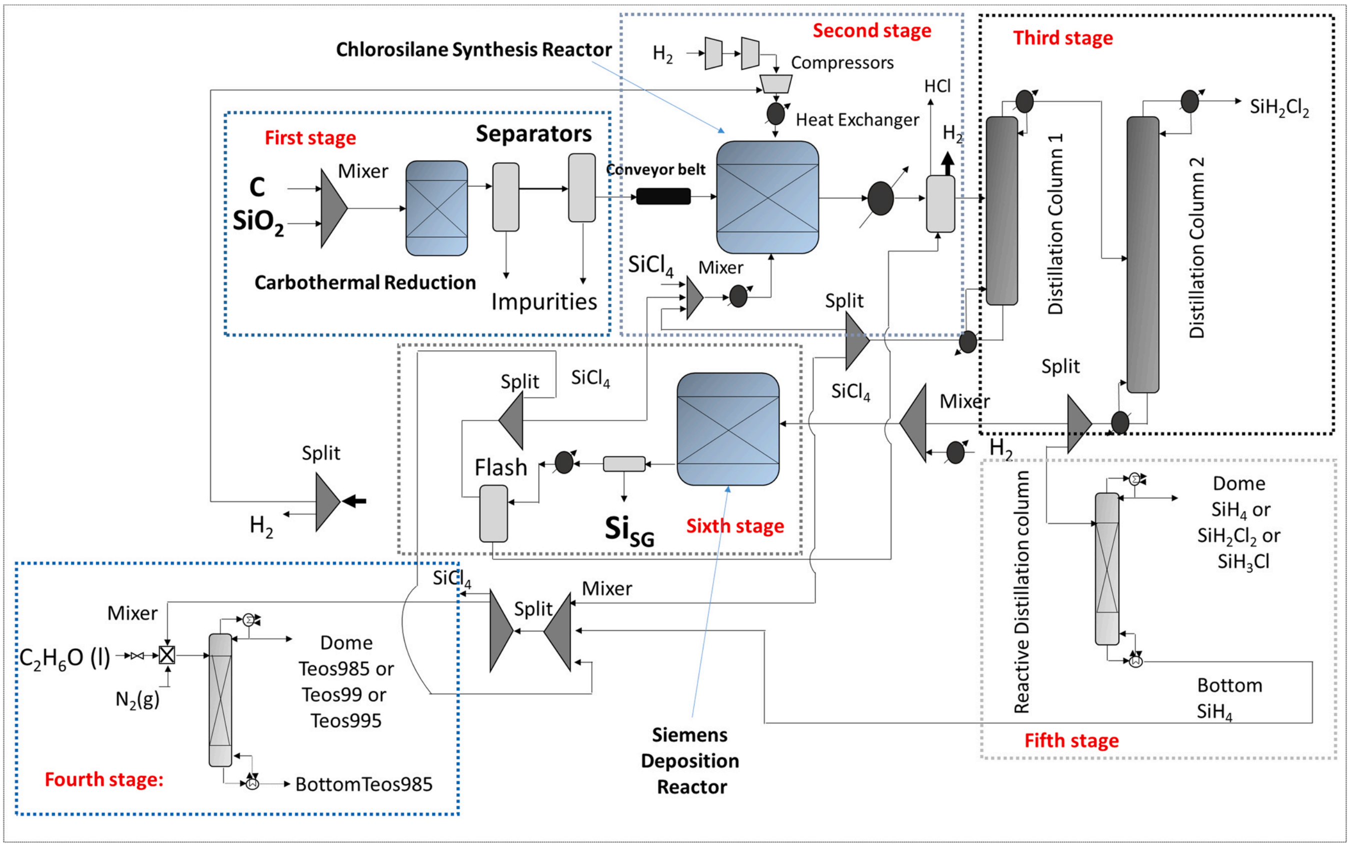

Fig. 2 – Flowsheet of the solar grade silicon multiproduct refinery.

Table 3 – Profit and Operating Costs for fairness approaches.

	Original	N	RW	SW
Constraint of M$20 in operating costs				
Profit [M$/y]	117.94	86.37	91.67	86.40
Operating costs [M$/y]	16.09	20.00	14.70	20.00
Constraint of M$15 in operating costs				
Profit [M$/y]	102.20	91.37	104.19	91.37
Operating costs [M$/y]	10.00	15.00	7.17	15.00
Uncertainty in Si_{SG} 10% above the actual cost				
Profit [M$/y]	123.28	96.86	115.20	96.90
Operating costs [M$/y]	15.67	20.00	16.66	20.00
Uncertainty in Si_{SG} 10% Below the actual cost				
Profit [M$/y]	101.12	75.87	84.79	76.00
Operating costs [M$/y]	8.60	20.00	11.09	20.00

2.1.1. *Model formulation*

The mathematical programming model to represent the multiproduct polycrystalline silicon facility was formulated as a nonlinear programming (NLP) problem. This model includes several variables and constraints to find the optimal design and operating conditions of the facility. Optimization can select the appropriate raw material feed flows, the production flows of any product, and the composition of each product. The complete model can be found in the Supplementary material section. It is important to mention that in the proposed model all the equipment in Fig. 2 must be included. Therefore, there are no constraints in the choice of any equipment.

For this approach, we propose to consider the main product (polysilicon) and byproducts (chlorosilanes) of the plant as the stakeholders of the system, since these products fulfill different demands, and the system goal is to maximize the satisfied demands. However, it is not trivial to do this simultaneously for all products because of economic constraints and issues in the formulation of the objective function, such as maximizing the profit of the system. To address this problem, we compare four objective functions to find the different individual productions and identify the most equitable.

The objective function of maximizing the system total profit, original hereinafter, is included as follows:

$$max\ w \tag{1}$$

$$w = S_{\text{polycrystalline silicon}} + S_{\text{byproducts}} - bRM - cE \tag{2}$$

$$S_{\text{polycrystalline silicon}} = Selling\ price\ of\ silicon\ {}^{*}Amount\ of\ silicon\ produced\ in\ a\ year \tag{3}$$

Here, the difference between the sales and costs related to the products are considered. Specifically, $S_{\text{polycrystalline silicon}}$ represents the sales of the main product (silicon), $S_{\text{byproducts}}$ is the sales of the byproducts, b is the unit cost of each raw material RM, and c is the cost of each utility E. The sales of high value-added byproducts include TEOS at different purities (99.5, 99, and 98.5), silane, dichlorosilane, and monochlorosilane.

$$S_{\text{byproducts}} = s_{\text{TEOS99.5}} + s_{\text{TEOS99}} + s_{\text{TEOS98.5}} + s_{\text{silane}} + s_{\text{dichlorosilane}} + s_{\text{monochlorosilane}} \tag{4}$$

Another objective function included in the analysis is based on the SW approach. This scheme seeks to maximize the sum of the sales of the stakeholders. Since the stakeholders of this system are different products, the SW scheme can be represented by the following formulation:

$$max\ x \tag{5}$$

$$x = s_{\text{TEOS99.5}} + s_{\text{TEOS99}} + s_{\text{TEOS98.5}} + s_{\text{silane}} + s_{\text{dichlorosilane}} + s_{\text{monochlorosilane}} \tag{6}$$

Furthermore, the RW approach is also evaluated as objective function. For this scheme, the smallest sales function is maximized. To represent this, the variable y is included and minimized subject to certain constraints:

$$min\ y \tag{7}$$

$$-s_{\text{TEOS99.5}} \le y \tag{8}$$

$$-s_{\text{TEOS99}} \le y \tag{9}$$

$$-s_{\text{TEOS98.5}} \le y \tag{10}$$

$$-s_{\text{silane}} \le y \tag{11}$$

$$-s_{\text{dichlorosilane}} \le y \tag{12}$$

$$-s_{\text{monochlorosilane}} \le y \tag{14}$$

The N scheme is the other objective function evaluated. In this approach, the sum of the logarithms of the sales of the stakeholders is maximized.

$$max\ z \tag{15}$$

$$z = \log s_{\text{TEOS99.5}} + \log s_{\text{TEOS99}} + \log s_{\text{TEOS98.5}} + \log s_{\text{silane}} + \log s_{\text{dichlorosilane}} + \log s_{\text{monochlorosilane}} \tag{16}$$

The methodology presented by Gutiérrez (2003) was used to calculate the operating cost of the process:

$$Operating\ costs = a \quad I_F + b \quad RM + c \quad E + d \quad MO - p \quad SP \tag{17}$$

where, a is a factor that considers annual expenses such as maintenance; I_F is the fixed annualized investment; b is the unit cost of each raw material RM; c is the cost of each utility E; d MO is the cost of manpower; p is the price of each byproduct SP. A detailed economic evaluation based on the procedure proposed by Turton et al. (2012) was carried out, estimating the equipment cost, production cost, maintenance, administration, and manpower. This considers the investment cost of a refinery with a capacity of more than

Table 4 – Operating conditions of each stage of the process for the constraint of M$20 in operating costs.

	TCa	Hy			Separation				Col RD TEOS						Col RD SiH_4 – SiH_2Cl_2 - SiH_3Cl						Siemens
					C1		C2		98.5		99.0		99.5		SiH_4		SiH_2Cl_2		SiH_3Cl		
	T [K]	T [K]	P [kPa]	$H_2/SiCl_4$	FR	RR	FR	RR	RR	P [kPa]	RR	P [kPa]	RR	P [kPa]	DFR	RR	DFR	RR	DFR	RR	T [K]
Original	2821	680.2	2026.1	1.99	2.16	15.99	7.82	63.21	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	N/A	N/A	N/A	N/A	1500.00
N	2806	675.3	2025.2	1.92	2.19	15.56	6.81	69.13	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1500.00
RW	2808	677.2	2026.5	1.98	2.18	12.34	5.45	60.03	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.50	25.8	1498.23
SW	2817	674.6	2026.5	1.92	2.15	37.67	6.82	90.01	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1489.62

*TCa=Thermal Carboreduction; Hy=Hydrochlorination Reactor; C1 = Column 1; C2 = Column 2; Col RD= Reactive distillation Column; T = Temperature; P = Pressure; FR= Feed Ratio; RR= Reflux Ratio; DFR=Distillate to feed ratio; N/A=Not apply.

15,000 tons per year of solar grade silicon, and 8500 tons per year of any other high value-added product. However, it is important to note that the change in operation does not change the cost of the equipment. Also, it is important to note that the storage costs of each product are not taken into account, since the market demand is expected to be covered according to the given solution.

3. Results

The study was considered under various scenarios: the first one with a refinery operating cost constraint of M$20 per year, the second one with a refinery operating cost constraint of M$15 per year, and the last two scenarios under the uncertainty of the solar grade silicon market price (i.e., 10% above and 10% below of the actual cost). The optimization of the different scenarios was implemented on the GAMS software. The code that contains the model of the Solar-Grade Silicon Refinery has around 2800 equations and 3750 variables and it is solved with the solver CONOPT as an NLP problem. The computing time to obtain the optimal solutions is around 30 min, using a computer with an Intel® Core™ i5–10505 processor and 8.00 GB of RAM.

It is evident that both the profit and the operating costs of each scenario, whether it is the original or each equity approach, vary. And even more important is that the manufacturing of each value-added product under each allocation scheme finds different solutions which could eventually favor market demands. Table 3 shows the profit and operating costs of the scheme without any equity approach (original), of the N, RW and SW approaches.

Within the first scenario, constrained by maximum operating costs of 20 [M$/y], it can be observed that the original scheme is the one with the highest profit (117.94 [M$/y]), even though it is not the one with the highest operating cost (the reason can be analyzed in Fig. 3a and Table S1 of the Supplementary material). Compared to the fairness approaches, the original scheme practically opts to produce solar grade silicon (1875 [kg/h]), forgetting to satisfy the demand for other products. In contrast, the N and RW fairness approaches can be observed. These schemes diversify the production of the refinery. With similar solar grade silicon production, the N and RW schemes (1800 and 1803 [kg/h], respectively) allocate TEOS production to its various purities (293.65 [kg/h] 99.5%, 286.84 [kg/h] 99.0%, 282.05 [kg/h] 98.5% and 31.53 [kg/h] 99.5%, 47.29 [kg/h] 99.0%, 78.827 [kg/h] 98.5%, respectively). The same production is suitable for chlorosilanes (79.01 [kg/h] silane, 1873.27 [kg/h] dichlorosilane, 218.324 [kg/h] monochlorosilane and 0.34 [kg/h] silane, 2572.62 [kg/h] dichlorosilane, 40.821 [kg/h] monochlorosilane, respectively). Both the N and RW fairness approaches allocate production, which would favor market demand. Table S1 of the Supplementary material shows that the highest sales of all refinery products come from the production of silane and solar grade silicon. The refinery's raw material and utility costs can be seen in Fig. 4a (electricity, refrigerants, and steam). Fig. 4a explains how the profit of the scheme without fairness approach (original) is the highest. This is because the costs for refrigerants and electricity decrease since the use of reactive distillation columns to produce any TEOS or chlorosilane were not required. In contrast, the process design under the N- fairness approach promotes products such as TEOS at any purity. It also promotes the three chlorosilanes, which results in

Tablee 5 – Operating conditions of each stage of the process for the constraint of M$15 in operating costs.

	TCa	Hy			Separation				Col RD TEOS						Col RD SiH_4 – SiH_2Cl_2- SiH_3Cl						Siemens
					C1		C2		98.5		99.0		99.5		SiH_4		SiH_2Cl_2		SiH_3Cl		
	T [K]	T [K]	P [kPa]	$H_2/SiCl_4$	FR	RR	FR	RR	RR	P [kPa]	RR	P [kPa]	RR	P [kPa]	DFR	RR	DFR	RR	DFR	RR	T [K]
Original	2855	678.7	2026.1	1.99	2.27	18.32	8.01	78.45	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	N/A	N/A	N/A	N/A	1499.00
N	2820	680.0	2025.2	1.93	2.15	15.97	6.30	70.93	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1500.00
RW	2819	680.2	2026.1	1.94	2.19	15.89	5.78	58.79	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.50	25.8	1500.00
SW	2819	681.6	2026.1	1.94	2.17	16.56	7.04	87.31	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1500.00

* TCa=Thermal Carboreduction; Hy=Hydrochlorination Reactor; C1 = Column 1; C2 = Column 2; Col RD= Reactive distillation Column; T = Temperature; P = Pressure; FR= Feed Ratio; RR= Reflux Ratio; DFR=Distillate to feed ratio; N/A=Not apply.

Table 6 – Operating conditions of each stage of the process for uncertainty in Si_{SG} 10% above the actual cost.

	TCa	Hy			Separation				Col RD TEOS						Col RD SiH_4 – SiH_2Cl_2- SiH_3Cl						Siemens
					C1		C2		98.5		99.0		99.5		SiH_4		SiH_2Cl_2		SiH_3Cl		
	T [K]	T [K]	P [kPa]	$H_2/SiCl_4$	FR	RR	FR	RR	RR	P [kPa]	RR	P [kPa]	RR	P [kPa]	DFR	RR	DFR	RR	DFR	RR	T [K]
Original	2867	680.1	2026.0	2.03	2.25	21.42	7.03	67.21	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	N/A	N/A	N/A	N/A	1500.00
N	2823	679.9	2025.1	1.95	2.17	15.99	7.20	75.98	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1500.00
RW	2845	680.0	2026.0	1.93	2.17	16.51	6.98	67.56	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.50	25.8	1500.00
SW	2821	680.2	2026.0	1.95	2.16	37.90	7.61	71.39	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1500.00

* TCa=Thermal Carboreduction; Hy=Hydrochlorination Reactor; C1 = Column 1; C2 = Column 2; Col RD= Reactive distillation Column; T = Temperature; P = Pressure; FR= Feed Ratio; RR= Reflux Ratio; DFR=Distillate to feed ratio; N/A=Not apply.

higher operating costs, and the lowest profit of the equity approaches (86.37 [M$/y]). The effect in the RW fairness approach is seen in the low TEOS production (at any purity) and the high energy consumption related to the production of dichlorosilane. Finally, the SW fairness approach, under this first scenario, chooses to produce a higher proportion of the products with the highest added value. Which in principle could mean a higher profit, however, due to the high consumption of utilities (Fig. 4a), the design does not find a balance and is one of the designs with the lowest profit (86.40 [M$/y]).

Once the previous results were obtained and analyzed, the operating cost constraint was changed to a maximum of M$15 per year. In the original approach, the limiting operating costs are M$15 per year. It is for this reason that the design is limited to operating costs of M$10 per year. This is because the design opts for solar grade silicon production with a small quantity of TEOS production at high purities. This means that the costs of the utilities of the reboiler and condenser of the reactive distillation column are limited, but as production drops, the profit decreases, which creates a low production, and a low profit. This variation was included to consider the influence it could have on the scenario in the manufacture of high value-added products, such as TEOS (different purities) and chlorosilanes, and in turn on the final profit of the refinery, which is to analyze whether the optimal design would now opt for the manufacture of other high value-added products in each fairness approach and without it. We can now visualize in Table 3 that the maximum profit is obtained in the RW fairness approach (104.19 [M$/y]), followed by the original design (102.20 [M$/y]). And the N and SW fairness approaches with equal profit (91.37 [M$/y]). The analysis and discussion in the present scenario are relevant, since, despite constraining operating costs, a profit is not as high as in the first scenario without a fairness approach. However, the other fairness approaches do manage to increase their profit, the most striking case being the RW which achieves 12.52 [M$/y]. The reason can be analyzed with Figs. 3b, 4b, and 4b. By constraining the operating costs, the optimal RW design allocates a higher production of TEOS 98.5% (121.59 [kg/h]) and silane (20.74 [kg/h]), which can be seen in Fig. 3b. This represents higher sales (Table S2 of the Supplementary material) for these products and in turn lower operating costs, specifically for the steam (1.88 [M$/y], compared to 4.21 [M$/y] in the original approach) used in the reboiler of the reactive distillation columns (Fig. 4b). In general, the fairness and original approaches tend to maintain the same principle, or the original to manufacture the largest amount of solar grade silicon regardless of the other products, the N and RW fairness approaches to diversify production, and the SW approach to choose for the lowest value-added product in terms of sales.

The other two scenarios were thought of in case the price of the main product, solar grade silicon, were to vary in its selling price by a 10% increase and a 10% decrease (all without constraints on operating costs). The results are interesting since the refinery without any (original) fairness approach tends to increase the profit (123.28 [M$/y]) by increasing the price of solar grade silicon and substantially decreasing it (101.12 [M$/y]) by reducing the price of solar grade silicon (see Table 3), as in the previous scenarios, Fig. 3c, d, 4c and, d show that the optimal design only cares about the production of solar grade silicon and practically no other high value-added products. This is reflected in the high

Table 7 – Operating conditions of each stage of the process for uncertainty in Si_{SG} 10% below the actual cost.

	TCa	Hy			Separation				Col RD TEOS						Col RD SiH_4 – SiH_2Cl_2- SiH_3Cl						Siemens
					C1		C2		98.5		99.0		99.5		SiH_4		SiH_2Cl_2		SiH_3Cl		
	T [K]	T [K]	P [kPa]	$H_2/SiCl_4$	FR	RR	FR	RR	RR	P [kPa]	RR	P [kPa]	RR	P [kPa]	DFR	RR	DFR	RR	DFR	RR	T [K]
Original	2819	671.3	2026.0	1.90	2.17	14.94	6.82	61.29	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	N/A	N/A	N/A	N/A	1488.12
N	2834	677.1	2024.0	1.91	2.17	15.18	6.81	60.13	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1489.17
RW	2837	678.2	2026.0	2.30	2.18	13.76	6.95	62.21	1.90	101.32	1.37	101.32	1.21	101.32	0.25	61.2	0.50	25.8	0.50	25.8	1481.45
SW	2821	674.9	2026.0	2.03	2.17	59.31	6.87	87.01	N/A	N/A	N/A	N/A	1.21	101.32	0.25	61.2	0.50	25.8	0.33	24.3	1499.98

*TCa=Thermal Carboreduction; Hy=Hydrochlorination Reactor; C1 = Column 1; C2 = Column 2; Col RD= Reactive distillation Column; T = Temperature; P = Pressure; FR= Feed Ratio; RR= Reflux Ratio; DFR=Distillate to feed ratio; N/A=Not apply.

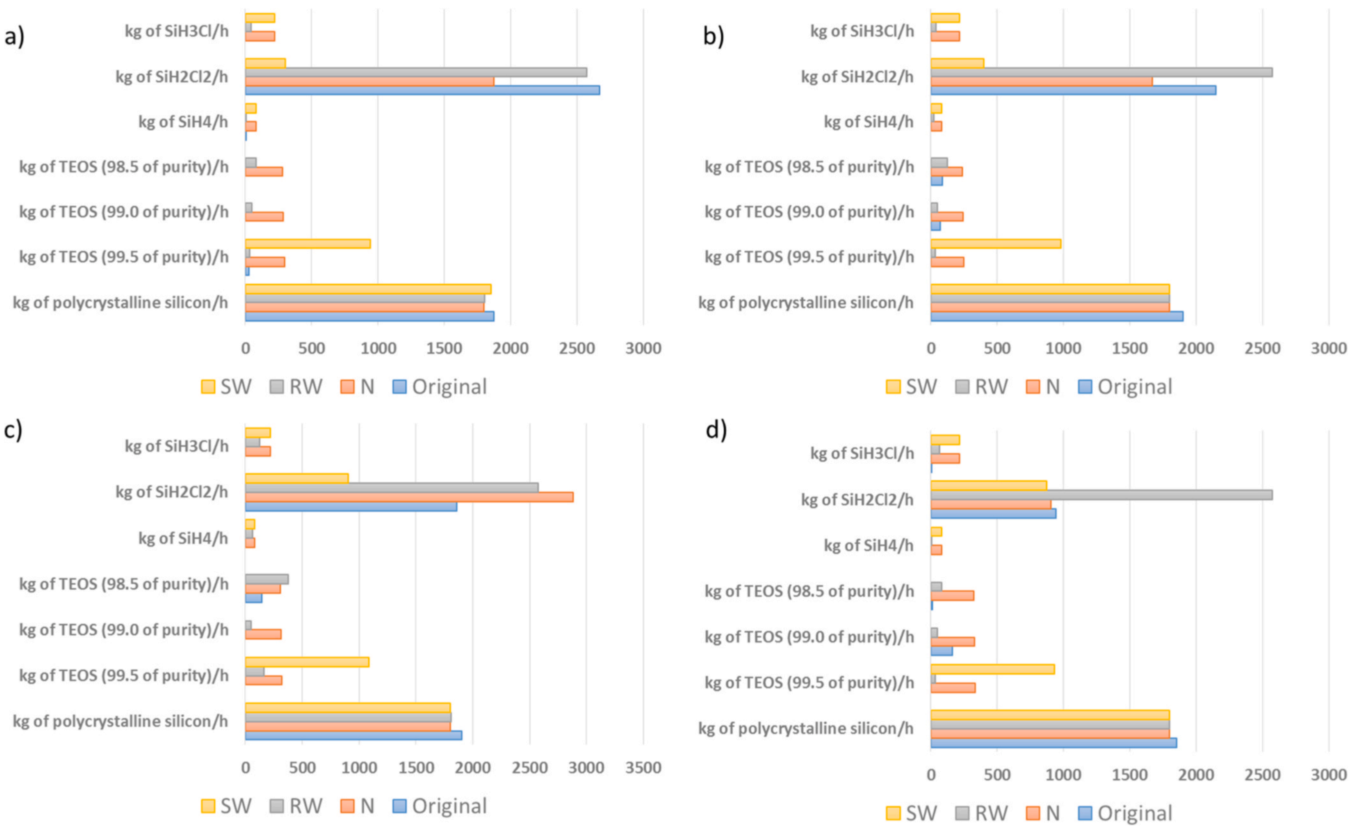

Fig. 3 – kg of solar grade silicon and other high value-added products generated by the refinery annually, under each fairness and non-fairness approach. a) Constraint of M$20 in operating costs, b) Constraint of M$15 in operating costs, c) Uncertainty in Si_{SG} 10% above, and d) Uncertainty in Si_{SG} 10% below.

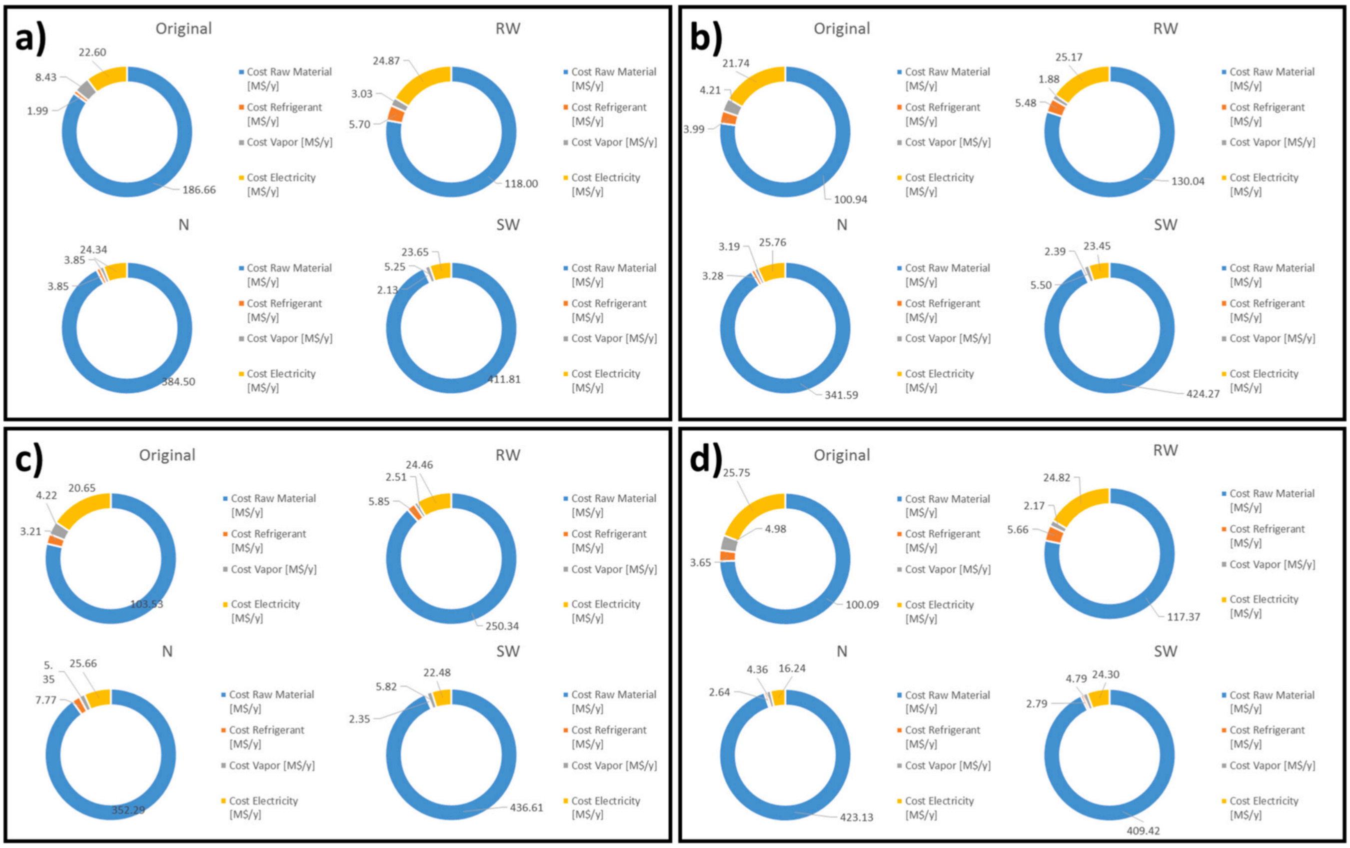

Fig. 4 – Costs of raw material, electricity, steam and refrigerant for each fairness and non-fairness approach. a) Constraint of M$20 in operating costs, b) Constraint of M$15 in operating costs, c) Uncertainty in Si_{SG} 10% above, and d) Uncertainty in Si_{SG} 10% below.

cost of electricity emanating from Siemens' deposition reactors, increasing the facilities of this item. The RW, N and SW fairness approaches maintain their behavior from the previous scenarios, as can be seen in Table 3. This means that the N fairness approach seeks to diversify production, even though there is uncertainty in the cost of the main product. On the other hand, the RW fairness approach increases its profit (115.20 [M$/y]) with a 10% increase in the present price of solar grade silicon and decreases it substantially (84.79 [M$/y]) with a decrease in the price of solar grade silicon. Finally, the SW fairness approach allocates high chlorosilane production (Fig. 3c and d), regardless of the high raw material cost this may represent (Figures 5c and 5d).

The final analysis and discussion when evaluating the different scenarios under the various fairness approaches can conduct us to reflect on the use of such fairness approaches in intensified processes. We generally tend to think that the use of any intensified equipment, by default, will help us to manufacture any product at a low cost, with low energy consumption, and in turn, this will help us to increase profit. This work, through the evaluation of the different fairness approaches in a highly intensified process, such as the solar grade silicon multiproduct refinery, helps us visualize that although equipment may seem favorable when intensified (in the case of the reactive distillation columns), it may be disadvantageous, and the operating costs may exceed the profit costs at a production point. In other words, the use of fairness approaches, apart from helping to diversify production in case the market demands some product, helped to show that the indiscriminate production of products such as TEOS or chlorosilanes in intensified equipment can be counterproductive, increasing operating costs and thus reducing the profit of the resulting design. In addition, the fairness approach that presented the greatest diversification was the N approach. It should be noticed that if it is required to supply the market with all the high value-added products, or only those that the market demands, the optimum design of each scenario and in each fairness approach (shown in Table 4–7, of the multiproduct refinery) can be used.

From the analysis of the design and operating conditions presented in Table 4 to 7, the equipment requires extreme conditions to meet the production requirements allowable within the operating and modeling ranges that can be found in the work of Ramírez-Márquez et al. (2020), practically all the designs presented go to the upper extremes, this can be seen in Fig. 4, where the utility costs are high. Therefore, it is recommended to use the design that diversifies production or the design with higher utility, depending on the required case.

4. Conclusions

This paper has introduced a systematic guide for the evaluation of fairness approaches in the design of multi-product industries. It has designed a process that considers optimal profit allocation and the manufacturing of multiple high value-added products. These players are part of an integrated system involving the production of solar grade silicon, TEOS (at different purities), and chlorosilanes (silane, dichlorosilane, and monochlorosilane). To design the intensified solar grade silicon multi-product refinery under the fairness approaches, a set of subrogated models of each unit was presented (where the material and energy balances are fulfilled). The results showed different optimal allocations for the economic functions under different circumstances (constraints on operating costs and uncertainty in solar grade silicon costs). Significant differences were observed in the allocation of products and profit under the fairness approaches. The differences in profit with each approach involved highlighted the importance of exploring and analyzing these possible allocations as they can be key for decision makers in considering whether to invest or not in a system and how to design it to meet the market demand. In those different scenarios, the optimal solution provided the best design; however, there was no specific scheme that can provide a design able to fulfill market demands and fluctuations. Furthermore, it was found that fairness approaches can decrease profit depending on the desired product, despite being manufactured in an intensified team. We found that larger profit designs avoid the use of intensified equipment due to high utility consumption. Moreover, each solution given by each approach provided a different design of the solar grade silicon multi-product refinery. In this sense, this work can form the basis for future research, especially for the design of multi-product industries involving competition between players, and only a single economic actor can be compared. It is interesting to note that the RW approach provided diversity in refinery output and high profit. Furthermore, using the N approach, we found an optimal design that allows the installation of the multi-product solar grade silicon refinery obtaining a diversification of products and that may be adequate to meet the market demand. We also observed that the RW approach favors the actor with the lowest utility, which corresponds to chlorosilanes.

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César Ramírez-Márquez: Conceptualization, Methodology, Validation, Results, Manuscript, Writing – original draft, Writing – review & editing, Funding acquisition. **Aurora del Carmen Munguía-López:** Conceptualization, Methodology, Validation, Results, Manuscript, Writing – original draft, Writing – review & editing. **Mariano Martín:** Conceptualization, Methodology, Validation, Results, Manuscript, Writing – original draft, Writing – review & editing. **Juan Gabriel Segovia-Hernández:** Conceptualization, Methodology, Validation, Results, Manuscript, Writing – original draft, Writing – review & editing. **José María Ponce-Ortega**: Conceptualization, Methodology, Validation, Results, Manuscript, Writing – original draft, Writing – review & editing, Funding acquisition.

Data availability statement

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.cherd.2022.03.041.

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