DECISION SUPPORT TOOL FOR THE POLYMER INDUSTRY USING MICROSOFT EXCEL SOLVER

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Abstract: The products of the chemical industry, which includes the polymer industry, are present in today's society, and the demand for these products continues to grow throughout the year. However, the sector is not keeping up with the demands and is suffering from a lack of investment and decision support tools. The objective of this project was to evaluate Excel as a decision support tool in the polymer industry. A database was optimized using the GRG nonlinear model in Solver. The results showed that Solver alone is not the suitable tool for the type of optimization studied, as it selects scenarios that do not meet the defined constraints. Therefore, the use of VBA or other more popular software should be evaluated

Keywords: Polymer industry; Petrochemical industry; Decision support tool; Excel.

FERRAMENTA DE SUPORTE À DECISÃO PARA A INDÚSTRIA DE POLÍMEROS UTILIZANDO MICROSOFT SOLVER EXCEL

Resumo: Os produtos da indústria química, que inclui a indústria dos polímeros, estão presentes no dia-a-dia da sociedade atual, e a demanda por estes produtos crescem ao decorrer do ano. Porém, o setor não está acompanhando as demandas e sofre com a falta de investimentos e ferramentas de apoio à tomada de decisões. O objetivo desse projeto foi avaliar o Excel como ferramenta de apoio à tomada de decisões na indústria de polímeros. Um banco de dados foi otimizado pelo solver, usando o modelo GRG não linear. Os resultados encontrados mostraram que o solver por si só não é a ferramenta adequada para o tipo de otimização estudada, por selecionar cenários que não atendem às restrições definidas. Sendo assim, deve-se avaliar o uso do VBA ou de outros softwares mais populares.

Palavras-chave: Indústria de polímeros; Indústria petroquímica; Ferramenta de apoio à decisões; Excel.

1. INTRODUCTION

Chemical industry products are present in various sectors of society's daily life, as they are found in transportation, objects, agriculture, healthcare, among others. This demonstrates that the chemical industry is strategic, as its products are found in diverse sectors, either as raw materials or intermediate goods. In 2021, the sector had a net revenue of US$ 142.8 billion, according to the *Anuário da Indústria Química Brasileira* (ABIQUIM) [1].

Delving further into the Brazilian scenario, 2021 witnessed the highest net revenue since 2014. However, it can be observed that the chemical industry is not growing in line with the demand. According to data from the 2021 Annual Performance of the Brazilian Petrochemical Industry by ABIQUIM, the sector presented a trade deficit of US$ 45 billion, surpassing the previous year's value of US$ 30.4 billion, marking a 48% increase [1].

The polymer industry is integrated within the structure of the chemical industry, and thus, it can be affected by the instabilities of the Brazilian market, potentially impacting investments in the sector. However, for investments to be made, different scenario simulations for the industry regarding prices, demand, technological routes, and constraints must be performed [1,2].

Numerous published works address decision support tools to assist the chemical sector in responding quickly to market instabilities. Afshar *et al.*, building upon a pioneering study conducted at the University of Wisconsin, advanced in research evaluating the development of a mathematical model to help the petrochemical industry cope with market instability and facilitate investments in the field [2].

The following modeling insights are described: The petrochemical industry consists of chemical processes; every chemical or physical process has its specific material flow, each of which is considered as an input in the technology catalog; material interactions in the process are linear, enabling representation of each process with an input or output matrix; each process has its limitations and supply-demand restrictions [2].

Some authors utilized the mathematical model developed by Afshar *et al.*, like Junior and Boaventura, who conducted studies on cost optimization in the Brazilian petrochemical industry. However, these authors did not focus on a specific branch of the petrochemical industry and used a quite robust software for the optimizations [2, 3, 4].

The objective of this work is to evaluate the use of a more accessible software, Microsoft Excel Solver, as a decision support tool in the polymer industry. Additionally, it aims to understand how variations in product demand impact the sector.

2. METHODOLOGY

In this work, the mathematical model described by equation 1, as discussed by Afshar *et al.* [2], was considered. The letter i refers to products, and j to processes, while N and M represent the total number of products and processes to be analyzed, respectively. P represents the price of product i, F is the supply limit of product i, C is the cost of process j, X is the capacity of process j, Q represents the quantity produced of product i, D is the demand for product i, and H is the burning price of product i. The letters B, S, and the factor aij refer, respectively, to the maximum capacity of process j, the maximum supply limit of product i, and the mass balance factor that relates product i to process j.

$$Cost\ of\ production: \sum_{i=1}^{N} P_i * F_i + \sum_{j=1}^{M} C_j * X_j + \sum_{i=1}^{N} (Q_i - D_i) * (P_i - H_i) \quad \textbf{eq. 1}$$

Subject to constraints:

$$X_j \geq 0 \quad \textbf{eq. 2}$$

$$X_j \leq B_j \text{A} \quad \textbf{eq. 3}$$

$$F_i \geq 0 \quad \textbf{eq. 4}$$

$$F_i \leq S_i \quad \textbf{eq. 5}$$

$$Q_i \geq 0 \quad \textbf{eq. 6}$$

$$D_i \leq Q_i \quad \textbf{eq. 7}$$

It is known that:

$$Q_i = Fi + a_{ij} * Xj \quad \textbf{eq. 8}$$

The 24 products studied in this work are, in the order of enumeration: 1,2-dichloroethane, terephthalic acid, benzene, butadiene, vinyl chloride, chlorine, styrene, ethane, ethylene, ethylbenzene, ethylene glycol, natural gas, methanol, m-xylene, naphtha, polyvinyl chloride, polystyrene, polyethylene, polyethylene terephthalate, polypropylene, propylene, p-xylene, soda, and toluene. These products were selected considering the polymer industry based on the structure described by Gomes *et al.* [4]. The data of the products and processes were collected from the work of Junior [3]. The processes involved are described in Table 1.

Tabela 1. List of processes [3].

j	PROCESSES	j	PROCESSES	j	PROCESSES
1	1,2-Dichloroethane via chlorination of ethylene	**14**	Ethylene via propane pyrolysis	**27**	PS via mass/suspension polymerization
2	Terephthalic acid, crude, via p-xylene	**15**	Ethylbenzene via benzene alkylation	**28**	HDPE via Union Carbide technology
3	Benzene via toluene disproportionation	**16**	Ethylene glycol via ethylene oxide hydration	**29**	HDPE via HOECHST technology
4	Benzene via toluene hydrodealkylation	**17**	Ethylene glycol via ethylene oxidation	**30**	HDPE via Stamicarbon technology
5	Butadiene via n-butane dehydrogenation	**18**	Methanol via natural gas (methane)	**31**	HDPE via Montedison technology
6	Vinyl chloride from ethylene	**19**	p-Xylene via m-xylene isomerization (aromax-isolene)	**32**	LDPE via autoclave reaction
7	Vinyl chloride via 1,2-dichloroethane	**20**	p-Xylene via m-xylene isomerization (parex-isolar)	**33**	LDPE via autoclave reaction (mixture)
8	Chlorine via electrolysis of sodium chloride	**21**	PVC via mass polymerization	**34**	PET from DMT and ethylene glycol
9	Styrene via ethylbenzene (dehydrogenation)	**22**	PVC via suspension polymerization	**35**	PET from terephthalic acid and ethylene glycol
10	Styrene via ethylbenzene (hydroperoxide process)	**23**	PVC via emulsion polymerization	**36**	PP via liquid-phase process
11	Ethylene via ethane-propane cracking	**24**	PVC via emulsion polymerization (batch)	**37**	PP via vapor-phase process
12	Ethane via naphtha cracking (high severity)	**25**	PS via mass polymerization	**38**	PP via slurry process
13	Ethylene via ethane pyrolysis	**26**	PS via emulsion polymerization	**39**	PP via solution process

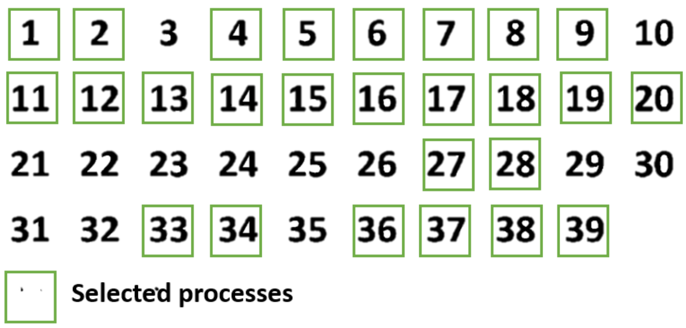
For the optimization process, Microsoft Excel Solver was used as the optimization tool. The selected objective function was the one containing the production cost formula. The variables considered were the supply limit and process capacity. The constraints were added according to equations 2-7. Finally, the nonlinear GRG model was selected as the optimization model in this work.

Based on the data input, the optimization was conducted in three different stages. The first stage used the data provided by Junior, the second stage considered a 30% lower demand, and the third stage considered a 30% higher demand. Subsequently, discussions about the results obtained were conducted [3].

3. RESULTS AND DISCUSSION

The following Figure 1 displays the processes that were selected for the optimization using the data collected from Junior [3].

Figure 1. Processes selected in the first optimization.



After the optimization, out of the 39 processes studied, 13 were discarded. Thus, in the scenario of the studied data, in order to achieve the lowest cost for the polymer industry while adhering to the defined constraints, 13 processes should be excluded from the investment focus.

Regarding the products, there are raw materials, intermediates, and final products. The term Q represents the mass balance of the product, meaning it considers everything that was consumed or generated. Therefore, raw materials and intermediate products may have a Q value equal to 0 due to the total consumption of everything that was supplied and generated.

The final products, which would be the polymers such as polyvinyl chloride, polystyrene, polyethylene, polyethylene terephthalate, and polypropylene, were not accepted by the optimization. These products were discarded because the demand exceeds the quantity produced. Analyzing the results, it can be observed that Excel Solver was not a good optimization tool. The constraint was not met, yet the products still had values, which should not have occurred.

During the optimization, Excel displays the message "Solver could not find a feasible solution" and presents a scenario. During optimization, there will be peaks of maximum and minimum. Therefore, it is possible that the scenario found is one of the minimum peaks but not the most ideal one. Figures 2 and 3 below show, respectively, the selected processes for a scenario with 30% lower demand and 30% higher demand.

Figure 2. Processes selected for 30% lower demand.

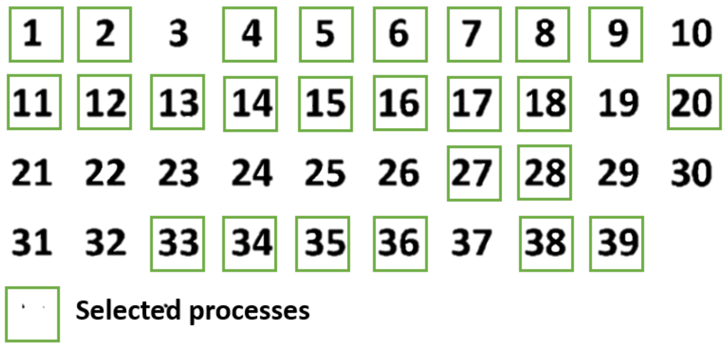
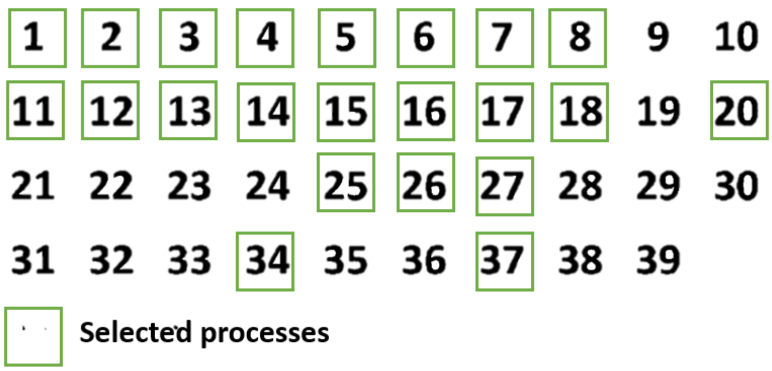


Figure 3. Processes selected for 30% higher demand.



For the 30% lower demand, 14 processes were discarded. In this situation, the accepted final products, considering those that met the constraints, were butadiene, chlorine, polyvinyl chloride, polystyrene, polyethylene terephthalate, and p-xylene. For the 30% higher demand, 17 processes were discarded. In this scenario, the only accepted products, considering those that met the constraints, are 1,2-dichloroethane, butadiene, polyvinyl chloride, polystyrene, and p-xylene. Due to the higher demand, it was expected that the number of discarded processes would increase.

The following Table 2 shows the cost values found for each optimization.

Tabela 2. Optimized cost found.

	Real data	30% lower demand	30% higher demand
Price (R$/ano)	41,751,716,422.925	45,136,539,743.603	2,763,807,923.491

The optimization with 30% lower demand resulted in the highest cost value, while the 30% higher demand led to the lowest cost value. When the demand is altered, some products and processes are discarded, while others may be accepted. There is no definite way to state that increasing the demand will always increase the price, as the variables for each product and process can behave differently.

Overall, the results show that Excel Solver cannot be used as a decision support tool for the polymer industry, as it did not achieve the proposed objective. The software fails to reach the optimal point, meaning it cannot select a scenario where all constraints are met and the lowest cost is achieved.

Analyzing Figures 1, 2, and 3 and the data obtained, it can be understood that more products and processes should have been discarded or accepted. Consequently, the total annual cost could have varied either up or down. The purpose of a decision support tool is to provide quick, clear results that help the user make informed decisions. However, the results obtained do not offer the required level of certainty.

4. CONCLUSION

The main objective of this project was to evaluate Excel Solver as a decision support tool for the polymer industry and to understand how the results behave with variations in demand. It can be concluded that, considering the proportion of data studied in this project, Excel Solver is not an ideal tool for data optimization.

Despite finding scenarios, the results obtained consider values of product and process parameters that should not be considered, thus failing to achieve the goal of a decision support tool, which is to provide more accurate data.

With the flexibility of demand, it can be observed that some products and processes may be accepted or discarded compared to the first scenario analyzed. However, due to the lack of accuracy, the comparison of results does not become clear.

Working with Excel Solver using VBA and establishing a more robust and rigorous structure may be a way to make Excel a promising tool for optimization problems at the level studied in this work. Additionally, other popular software tools, such as Python, can also be considered for analysis.

5. REFERENCES

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