Multi-Objective Sustainable Planning of Chemical Production Chains

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Abstract. Sound management of chemicals is one of key contributors for achieving the Sustainable Development Goals. The aim of this work is developing a multi-objective planning framework on the early planning and decision-making for chemical production processes, in order to obtain the maximum economic benefits, minimize the risk of possible chemical accidents to people, and minimize the environmental risk of production routes. GM (1, 1) model was established to predict the price trend and demand change of chemical products from 2020 to 2030. Combining three objective functions with the production chain constraints, a mixed integer linear programming model is developed. Polyvinyl Chloride production chains are taken as an example.

1. Introduction
Petroleum and chemical industry is the basic strategic industry of national economy and one of the pillar industries in China. As of December 2019, there were 26271 Enterprises above Designated Size in the petroleum and chemical industry. The number is up 4.8% over last year. The operating revenue of the petroleum and chemical industry was 12.27 trillion yuan, an increase of 1.3% over last year, accounting for 11.6% of the national scale industrial operating income [1]. After years of rapid development of China's chemical industry, the contradiction of internal accumulation is becoming more and more prominent. Chemical industry parks (CIPs) have become the mainstream of the development of chemical industry. The healthy and sustainable development of chemical industry park is facing unprecedented pressure [2]. The early planning and decision-making of chemical product chain in the park is very important. Through the feasibility analysis of economy, technology and environment, the product chain structure suitable for regional economic development is determined [3]. The final products are determined according to the market and price, and the coordination of three objectives with economic, safety and environmental performance in production is considered.

The prices of chemicals are affected by raw materials, domestic and foreign markets, and output. It can be regarded as a grey system. GM (1, 1) is a common analysis model of grey system [4-8]. Multi-objective decision making is the process of making a scientific and rational choice between multiple conflicting objectives. The route choice of chemical products requires comprehensive consideration of multiple factors, while the method of multi-objective decision can balance multiple contradictory goals [9-16].

The above research is aimed at the research of chemical product chain, considering many factors. However, there is a lack of the impact of a certain indicator change on the specific results. If the market demand and raw material supply will have an impact on the price changes of chemicals, the price changes will lead to economic factors. In this paper, GM (1, 1) model is established to forecast...
the output of the chemicals from 2020 to 2030. The relationship between output and price is analyzed, and the Fourier function between output and price is obtained, so as to obtain the price of the chemicals in 2020-2030. Secondly, a mixed integer linear programming (MILP) model was established with economic, safety and environmental criteria. Through a comparative analysis of the solutions under the three scenarios, it is possible to achieve economic efficiency while taking into account safety and environmental performance.

2. Methodology

2.1 Price projections

PVC is widely used in building materials, chemical, electronic, medical, food and other industries\cite{18}. Domestic demand for PVC is increasing year by year, and the price is also changing. Therefore, the analysis and forecast of PVC market and price trend can help us to grasp the market situation and plan the production\cite{19}.

In order to forecast the PVC production from 2020 to 2030, GM (1, 1) prediction model was established. The known reference sequences are as follow: \(X(0)(k) = [x(1), x(2), \ldots, x(N)]\). The sequence of one-time accumulation is as follows: \(X(1)(k) = \sum_{i=1}^{k} x(i)\), \(Y(1)(k) = \frac{x(i) + x(i+1)}{2}\). Then we can get the equation:

\[
X(0)(k) + aY(1)(k) = b;
\]

\[
X(0)(k + 1) = (1 - e^a) \left( x(1) - \frac{b}{a} \right) e^{-ak}.
\]

We can get \(a = -0.0848\), \(b = 9.1235\). The formula of production prediction function is as follows: \(X(0)(k + 1) = (1 - 0.9187) \times (x(0)(1) + 107.5884) \times 1.0885^k\), where \(k\) is the year. Therefore, the output of PVC in China from 2020 to 2030 can be obtained.

Fourier function can be used to characterize the price change of chemical products\cite{12}. Therefore, Fourier analysis is used to analyze the relationship between price and output. Therefore, the functional relationship between price and output can be obtained: \(y = a0 + a1 \times \cos(x \times w) + b1 \times \sin(x \times w)\), where \(a0 = 7212, a1 = 1191, b1 = 475.1, w = 8.855\).

The relation between yield and year, price and output is obtained, and the relation between price and output is obtained by taking output as connection. Then we can get the price corresponding to the year. The forecast price can provide some insights for the actual production, and make targeted selection and change according to the market changes.

2.2 Route selection under optimization

Chemical reaction program planning is highly complex and important in chemical industry. Each route has its own advantages, but due to different objectives, there are inevitably deficiencies. Therefore, it is very important to determine the response path of high economic efficiency, high security and low environmental risk in the early stage of planning. In this section, a MILP model is established by combining the economic benefits, safety and environmental objectives with the relevant constraints of the production chain.

2.2.1 Definition of objective function

(1) Economic Goals:

Economic benefits can be expressed by calculating incremental net present value, incremental internal income value, cash flow discount rate and economic value added\cite{20,21}. In the early stages of planning, there is a lack of sufficient information to conduct a complete economic benefit assessment.
For its simplicity, economic value added is chosen as the evaluation index. Use the following formula to calculate:

\[ ECO = \sum_j \sum_i o_{ij} c_i x_i \]

(2) Safety Goals:
Safety objectives can be transformed into safety risk index to measure. Al-Sharrah\(^{[22]}\) proposed a safety index, which is based on the multiplication of the potential number of people affected by chemical leakage, accidents occurred in the process of chemical production and the number of main processes in the production process. It can be calculated by the following formula:

\[ SAFE = \sum_j \sum_i o_{ij} k_i Inv_{ij}, \quad k_i = Freq_i \times Haz_i \times Size_{ij} \]

(3) Environmental Goals:
Environmental issues have now become an important consideration due to the potentially harmful effects of chemical release. The Indiana Relative Chemical Hazard Score (IRCHS) is comprehensive, including water hazard value, air hazard value, land hazard value, global hazard value and environmental hazard component of health impact hazard value, exposure hazard value and safety hazard value\(^{[6]}\). Use the following formula to calculate:

\[ ENV = \sum_j \sum_i o_{ij} (IRCHS_i \times x_i) \]

2.2.2 Planning Model
Model constraints
(1) Mass balance: \( F_i + \sum_{j=1}^{M} o_{ij} x_i = Q_i \), \( i = 1,2,\ldots,N \)
(2) Final products yield: \( Q_i \leq D_j U_i \), \( i \in I_1 \)
(3) Productivity of chemical process: \( B_j Y_j \leq x_j \leq HY_j \), \( j = 1,2,\ldots,M \)
(4) The number of chemical process: \( \sum_j Y_j \leq 1 \), \( j \in J_1 \)
(5) The number of final products: \( \sum_j Y_j = P \), \( j \in J_2 \)
(6) Supply number of feed stocks: \( F_i \leq S_i \), \( i \in I_2 \)
(7) Capital budget: \( \sum_{j=1}^{M} Cap_j \times Y_j \leq Bg \)

2.3. Solution method

2.3.1 Solving under single goal
In this scenario, only one function will be considered. The optimization function is as follows:

\[ \max (ECO) = \sum_j \sum_i o_{ij} c_i x_i \]  \hspace{1cm} (1)

\[ \min (SAFE) = \sum_j \sum_i o_{ij} k_i Inv_{ij} \]  \hspace{1cm} (2)

\[ \min (ENV) = \sum_j \sum_i o_{ij} (IRCHS_i \times x_i) \]  \hspace{1cm} (3)

2.3.2 Solution under the ε-constraint optimization
If one of goals is chosen as the most important consideration, then the other two goals become constraints. In this scenario, the economic goal is taken as the optimization function, and the safety and environmental goals are the constraints. The optimization function is as follows:

Objective function:

\[ \max (ECO) = \sum_j \sum_i o_{ij} c_i x_i \]  \hspace{1cm} (4)

Constraint condition:

\[ SAFE = \sum_j \sum_i o_{ij} k_i Inv_{ij} \leq \varepsilon 1 \]  \hspace{1cm} (5)

\[ \min (SAFE) \leq \varepsilon 1 \leq \max (SAFE) \]
\[ ENV = \sum_{i}^{M} \sum_{j}^{N} a_{ij} (IRCHS_{i} \times x_{i}) \]  
\[ \min (ENV) \leq \varepsilon 2 \leq \max (ENV) \]  
\[ e_{(ECO)}(j) \leq \frac{ECO^{u}_{j} - ECO^{l}_{j}}{ECO^{u}_{j} - ECO^{l}_{j}} \]  
\[ e_{(SAFE)}(j) \leq \frac{SAFE^{u}_{j} - SAFE^{l}_{j}}{SAFE^{u}_{j} - SAFE^{l}_{j}} \]  
\[ e_{(ENV)}(j) \leq \frac{ENV^{u}_{j} - ENV^{l}_{j}}{ENV^{u}_{j} - ENV^{l}_{j}} \]  

2.3.3 Solving under fuzzy optimization

On the basis of fuzzy optimization, a variable \( e \) is introduced to express satisfaction. Each goal satisfaction \( e \) is constrained by the following formula:

The value range of satisfaction \( e \) is 0-1, and the optimal path should make the satisfaction of the three objectives maximum. The objective function of fuzzy optimization can be expressed as follows:

\[ \max (z) = e_{(ECO)} + e_{(SAFE)} + e_{(ENV)} \]  

3. Case study

According to the references and relevant information, the reaction route was determined, as shown in Figure 1. There are 16 kinds of chemical substances in the production process, such as methane, acetylene, ethylene and PVC. The final model is a MILP model. The model has 23 continuous variables \( X_{i} \), 23 binary variables \( Y_{j} \), 13 constraints and 3 objective functions. The output co-efficient \( o_{ij} \), the price of the chemical product \( C_{i} \), the safety index \( k_{i} \), and other relevant data can be obtained [15]. GAMS software is used to solve the model.

4. Results and discussions

4.1 Solving under single objective

Through Eqs. (1)-(3) and taking different prices (2020, 2025 and 2030) of the final product PVC price in the forecast, a single target solution is obtained. The index values of each objective are shown in Figure 2. Figure 2 shows that the economic efficiency index of the PVC production chain is influenced by the final price of PVC. The economic benefit in 2025 is \( 1253.551 \times 10^{8} \text{S} \cdot \text{year}^{-1} \), which is very low compared to the economic benefit generated in 2020 and 2030. The safety and risk indices are the same in all three years of the search process, because we have chosen the same production routes. When comparing the solutions under the three different indexes, we can derive the optimal values for each index: the maximum value of economic efficiency is \( 55997.730 \times 10^{6} \text{S} \cdot \text{year}^{-1} \), the minimum value of safety risk is \( 958.738 \text{person} \cdot \text{year}^{-1} \), and the minimum value of environmental risk IRCHS is \( 36886.515 \). The above values (bold) are used as the optimal values of the solution index.
4.2 Solution under the $\varepsilon$-constraint optimization

By using the function (4) and the constraints (5) and (6), the objective values under the $\varepsilon$-condition are obtained. The maximum and minimum value of safety and environmental risk index is calculated, and its five equal parts are divided. Figure 3 shows that as the constraint value increases, the values of the three indicators increase as well. However, the safety risk index values total the same as the $\varepsilon$-constraint values. The results show that under the $\varepsilon$-constraint, it is possible to increase the economic efficiency with the safety and environmental risks that can be taken. However, the safety risk is greater than the environmental risk, which has a greater acceptable range than the environmental risk.

4.3 Solution under fuzzy optimization

By solving with the objective function (10) and additional constraints (7)-(9), the solution under fuzzy optimization can be solved. We can derive the optimal values for each index: the maximum value of economic efficiency is $36534.449 \times 10^4 \text{ S \cdot year}^{-1}$, the minimum value of safety risk is $1110.331 \text{ person \cdot year}^{-1}$, and the minimum value of environmental risk IRCHS is $54628.709$.

4.4 Discussion

Based on the above solution results, Figure 4 is obtained that considers multiple criteria. It can be seen
from Fig. 4 that when the safety and environmental risk values are small, the economic benefits are realized on the surface in a lighter color. This means that the value of economic benefit is small. Therefore, it is crucial to harmonize the contradiction among the three indicators. In order to facilitate the comparison of the values of each indicator, the maximum and minimum values of the three objectives can be obtained by solving the three functions, see Table 1.

We can obtain a fuzzy optimization scenario that improve weighs the economic, safety and environmental indicators. The values of the individual indicators are not particularly outstanding compared to the other scenarios. Comparing optimal solutions from single objective and $\varepsilon$-condition, we can conclude that the values of the indicators under the scenario solution are between the limit values (maximum and minimum) and do not deviate to a certain limit value. Therefore, the solution value under fuzzy optimization is considered to be the optimal Pareto solution.

When solving under a single objective and constraint, it is always important to have a comparison of the importance of the three indicators that will be economic, safety and environmental. For example, in a single objective scenario, three objectives are considered as the most important factors, respectively. Only one of them is selected for consideration, while the other two have no related constraints and limitations. Therefore, a solution with only one objective optimization is obtained. Also for the solution scenario under the $\varepsilon$-constraint, when economic objective is considered as the most important factor, then safety and environment are used as constraints. However, for the current development status of the chemical industry, we should not only consider one of them, but get the optimal value under the condition of taking all three into consideration. For fuzzy optimization, this situation is reasonably solved by introducing the satisfaction degree $\varepsilon$. The objective is to obtain the optimal value under the maximum satisfaction degree by applying fuzzy constraints to each target. The optimal value can be obtained when the satisfaction degree of the three targets is the highest at the same time, so that the three indicators are well considered with the same importance degree. Under fuzzy optimization, each indicator will not get the extreme value. We can select the reaction route: 10-18-22-19.
Table 1. Maximum and minimum values for three objectives

| objective | Economic (10^4 $ \cdot \text{year}^{-1}) | Safety (\text{person} \cdot \text{year}^{-1}) | Environment (IRCHS) |
|-----------|----------------------------------------|---------------------------------------------|---------------------|
| Minimum   | 25703.866                              | 958.738                                     | 36939.515           |
| Maximum   | 55997.730                              | 2185.2                                      | 107512.692          |

The production process of calcium carbide acetylene PVC (j=2, 23) has been replaced by ethylene method (j=18, 17 and 21) in developed countries. According to the characteristics of resource distribution, PVC industry pattern for calcium carbide method accounted for 80%, ethylene method accounted for 20%. The calcium carbide process for the mainstream of PVC industry. In addition, the calcium carbide PVC is a high carbon dioxide emissions industry. According to the statistics, the energy consumption of the whole process of domestic calcium carbide PVC production is 20.4% higher than that of ethylene PVC production. Therefore, in the current development of low-carbon economy background, calcium carbide PVC will also encounter some constraints on the policy.

5. Conclusion
A mixed integer linear programming model is proposed by combining price estimation, production process constraints, and objective functions. Three objectives include economic, safety, and environmental performances. The final solution under multi-objective fuzzy optimization is in line with the concept of a sustainable chemical product chain, balancing economic, safety and environmental risks.

Symbol Description

- \( B_j \): Minimum capacity of process j, 10^3 t/yr
- \( B_g \): Available budget, $ 
- \( Cap_j \): Total amount of funds for process j, $ 
- \( C_i \): Cost of chemical i, $ 
- \( D_i \): Market demand of chemical i, 10^3 t/yr 
- \( F_i \): The annual amount of chemical i available as a raw material, 10^3 t/yr 
- \( Freq \): Frequency of accidents, number of accidents per year 
- \( H \): Valid upper bound on production rates, 10^3 t/yr 
- Haz: Hazard of chemical, people affected per ton of chemical released 
- \( Inv \): Inventory of chemical released, t 
- \( IRCHS_i \): Indiana Relative Chemical Hazard Score of chemical i 
- \( J_1 \): The group of processes that produces a single chemical 
- \( J_2 \): The group of processes that produces the final products 
- \( M \): Total number of chemical processes in the programming model 
- \( N \): Total number of chemicals in the programming model 
- \( O_{ij} \): Output coefficient of chemical i from process j 
- \( P \): Number of the desired final product from the list of products 
- \( Q_i \): Annual amount of chemical i produced, 10^3 t/yr, for intermediate products, \( Q_i = 0 \) 
- \( S_i \): Supply availability of feedstock chemical i, 10^3 t/yr 
- \( Size_j \): Size of plant, number of major processes in process 
- \( U \): Upper limit of the market share, % 
- \( X_j \): Annual productivity of chemical process j, 10^3 t/yr 
- \( Y_j \): Binary variable for process j. if process j is selected, \( Y_j = 1 \), otherwise, \( Y_j = 0 \)

References

[1] Zhu, F. (2020) Review and Prospect of Economic Operation of China’s Petroleum and
Chemical Industry. Petroleum & Petrochemical Today, 28:1-8.

[2] You, W., Li, Z.G. (2020) Analysis of the Current Situation of China's Chemical Industry Parks and Proposals for Development Quality. Yunnan Chemical Technology, 47:159-161.

[3] Machado, M.C., Vivaldini, M., De Oliveira, O. J. (2020) Review Production and supply-chain as the basis for SMEs environmental management development: A systematic literature review. J. Clean. Prod, 273:123-141.

[4] Zhou, W., He, J.M. (2013) Generalized GM (1,1) model and its application in forecasting of fuel production. APPL MATH MODEL, 37:6234-6243.

[5] Wang, Z. X., Lin, Q., Pei, L.L. (2018) A seasonal GM (1,1) model for forecasting the electricity consumption of the primary economic sectors. Energy J, 154:522-534.

[6] Chen, J. Q. (2019) Fault Prediction of a Transformer Bushing Based on Entropy Weight TOPSIS and Gray Theory. Comput Sci Eng, 21:55-62.

[7] Wang, Z. G., Huang, L. F., He, C. X. (2019) A multi-objective and multi-period optimization model for urban healthcare wastes reverse logistics network design. J Comb Optim, 23:1-19.

[8] Xu, Q. W. Xu, K. L. (2020) Statistical Analysis and Prediction of Fatal Accidents in the Metallurgical Industry in China. INT J ENV RES PUB HE, 17:3790-3811.

[9] Jakob, B., Norbert, A. (2014) Multi-Objective Optimization and Decision Support in Process Engineering-Implementation and Application. CHEM-ING-TECH, 86:1065-1072.

[10] Gade P. R., Feng. Z.M. (2020) Multi-Objective Optimization Applications in Chemical Process Engineering: Tutorial and Review. PROCESSES, 8:508-540.

[11] Ghanima, A.S., A. Elkamel, A. Alyaa Aboud. (2010) Sustainability indicators for decision-making and optimization in the process industry: The case of the petrochemical industry. CHEM ENG SCI, 65:1452-1461.

[12] Jia, X. P., S.W. Wan. (2011) Multi-objective modeling and planning for the selection of chemical reaction routines. Energy Procedia, 14:649-654.

[13] Weng, H.L., H. Mimi H, H. Markku. (2012) Fuzzy Optimization for Screening of Sustainable Chemical Reaction Pathways. Italian Association of Chemical Engineering, 29:529-534.

[14] Juliana, S.E., D.M. Paulo C. (2016) Multi-criteria Decision Analysis for the Selection of Sustainable Chemical Process Routes During Early Design Stages. Chem Eng Res Des, 113:1-42.

[15] Eduardo, J.S., R.Q.R. Juan. (2018) Synthesis, design and optimization of alternatives to purify 2, 3-Butanediol considering economic, environmental and safety issues. Sustain Prod Consump, 11:282-295.

[16] Shin, Y.T., B.C. Kian. (2019) A Hybrid Multi-Objective Optimization Framework for Preliminary Process Design Based on Health, Safety and Environmental Impact. PROCESSES, 7:200-219.

[17] Bai, H.D. (2012) PVC Market Situation in China. Polyvinyl Chloride, 40:1-4.

[18] Liu, Y.J., C.B. Zhou, F. Li, H.J. Liu. (2020) Stocks and flows of polyvinyl chloride (PVC) in China: 1980-2050. Resour Conserv Recycl, 154:104584-104592.

[19] Mohamad, O. R., Jens-Uwe, R., Gunter, W., Huang, Y. L. (2010) A modular approach to sustainability assessment and decision support in chemical process design. Ind. Eng. Chem. Res, 49:7870-7881.

[20] Chen, X., Fu, W., Ji, Q. C., Li, S.W. (2019) Research on economic benefit evaluation method of integrated energy service renovation projects. Hubei electric power, 43:42-48.

[21] Ghanima, A .S. (2006) Planning the petrochemical industry in Kuwait using economic and safety objectives. Loughborough University.