Synthesis of C-H-O Symbiosis Networks Based on i-safe Index

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Abstract: The synthesis of C-H-O symbiosis network is considered in EIPs to reduce the amount of raw materials and waste discharge by using internal sources. In the conceptual design stage of C-H-O symbiosis networks, the concept of inherent safety index is introduced and safety factors are considered. Synthesis of C-H-O symbiosis networks based on i-safe index is proposed. Super-structure of C-H-O symbiosis networks was configured in EIPs, then optimization formulation was devised. A nonlinear programming (NLP) optimization model was established. A case study in Guizhou province shows that the method is useful in process decision-making, which could provide data support for early process decision making.

1 Introduction

Resource conservation is an important aspect to realize social sustainable development. In recent years, EIPs has become the focus of chemical enterprises. It is composed of a number of adjacent factories, which improve the environmental, economic and social performance of the chemical process through integrated measures such as the exchange of wastes or by-products between factories and the sharing of central public system [1].

The academic community has conducted a lot of comprehensive studies on EIPs. Roddy [2] reduced the carbon footprint of industrial processes by establishing a syngas network in EIPs. Lee [3] et al. proposed a two-stage EIPs water network optimization model suitable for continuous and intermittent unit operation modes. Lopez-diaz[4] et al. optimized the EIPs water network to reduce the environmental impact of factory waste water discharge into the river basin. Alnouri [5, 6] et al. designed EIPs waste water regeneration and reuse network by considering similar pipeline combination. Ubando [7] et al. established a mixed-integer nonlinear Programming model (MINLP) to select future plants, which reduced the environmental footprint of EIPs and optimized the annual profits of all companies. Ng [8] et al. proposed a fuzzy optimization method for palm oil processing plants involving multiple EIPs owners. Deng chun [9] et al. constructed the superstructure of purification and reuse hydrogen system among plants in the petrochemical park.constructed the superstructure of purification and reuse hydrogen system among plants in the petrochemical park. C-H-O Symbiosis Network (C-H-O SYN) synthesis is an important research direction of quality integration [1].Noureldin and el-halwagi [10] introduced a simplified method of multi-scale atomic calibration and design of C-H-O symbiosis network. Inherent safe design method can consider the safety factor in the early
stage of chemical process design and eliminate or reduce accidents in chemical and chemical industry from the source. It is important to improve the security of the whole life cycle. Safe design is integrated into the concept of C-H-O symbiosis network synthesis, considering safety of C-H-O symbiosis network optimization design method, taking an industry in Guizhou province as an example, illustrates this method can get good C-H-O symbiosis network security, to get the early in the process of security process provide effective methods.

2 Synthesis of C-H-O symbiosis networks based on i-safe index

Synthesis of C-H-O symbiosis networks is proposed, as shown in Fig.1.

![Synthesis of C-H-O symbiosis network based on i-safe index.](image)

3 Identify inherent safety index

Different inherent safety index were using in different chemical process, such as PIIS, ISI, i-safe, EHS, PRI, PSI, ICPRI, I2SI, Inherent safety index based on fuzzy theory, IBI, SWeHI, DHI etc. I-safe inherent safety index has attracted wide attention due to the small amount of data required and the fact that it can be applied in the conceptual design stage of process design. By comparing existing essential safety evaluation indexes, i-safe index is selected as the optimization index to measure the safety performance of the process. The i-safe index is divided into material index and process index. The material index includes NFPA reaction level, flammability, toxicity, and explosivity. The process indexes include reaction temperature, reaction pressure, yield and reaction heat.
4 Mathematical model

The comprehensive problem of C-H-O symbiosis network can be described as follows: given an EIPS containing several plants, a series of sources and sink exist in EIPs. The waste or by-product containing C-H-O atom with a fixed flow rate is the internal source, which can be used by the sinks in the park directly or after treatment. The sinks require a fixed flow rate for the input of raw materials, and external sources can be purchased to supplement the internal sources. External source is the raw materials purchased at the market. The new facility in EIPs for processing and distributing various internal sources and external sources is called intercept network. The intercept network consists of one or more interceptor that can separate, mix, chemically transform, heat, cool, pressurize, and decompress external and internal sources and distribute them to different sinks. Unused stream are discharged as waste. The goal is to obtain the economically optimal C-H-O symbiosis network of EIPs by certain optimization design method on the premise of satisfying the process constraints such as the actual feed ratio of the interceptor, impurity composition, yield and feed composition of the sink.

4.1 Superstructure C-H-O symbiosis network

The mathematical programming method is adopted to conduct the synthesis of C-H-O symbiosis network based on C-H-O symbiosis network superstructure in EIPs. The superstructure of C-H-O SYN is shown in Fig. 2.

![Figure 2. The superstructure of C-H-O SYN.](image)

where, the left circles are sources in EIPs, including internal sources and external sources, the right rectangles represent sinks, the middle boxes represent the interceptor. The potential distribution and allocation of sources to sinks may be represented it. In addition to the direct allocation of the source to the sink, the superstructure also contains the flow unit assigned to the interceptor for processing by the external source. External resources are allocated to the sink which processed by the interceptor. Unused external sources discharged as waste. It can be seen from the superstructure that the units in the EIPS are connected with each other through the material reuse flow, so as to save the resources. While the interceptor with the regeneration function realizes the centralized operation of internal and external sources in EIPs. The superstructure contains all the possibilities for the distribution of stream in EIPs.

4.2 Establishment of mathematical model

Based on the superstructure of C-H-O symbiosis network in EIPs in Fig. 2, the corresponding mathematical model was established. The streams are represented by continuous variables, and the model is Nonlinear Program (NLP) model. The inherent safety index value is related to the operating conditions of each interceptor and the
reactants, intermediates and products involved. The safety index is taken as a function of the stream to determine the optimal interceptor network. The minimum average i-safe index value of all interceptor elements in C-H-O symbiosis network is taken as the objective function to obtain the optimal safety C-H-O symbiosis network in EIPs.

The lower the OSI index value is, the better the security performance of the process is.

1) constraints

- **Source mass balance:**
  \[
  F_{SRi} = \sum_j F_{SRj,SKj} + \sum_k F_{SRj,REGk} + F_{SRj,WD} \quad \forall i
  \]

- **Interceptor inlet mass balance:**
  \[
  F_{REk} = \sum_i F_{SRi,REk} + \sum_e F_{SRe,REk} + \sum_n F_{REGn,REk} \quad \forall k, k \neq n
  \]

  where, \( F_{REk} \) is the flow of unit inlet.

- **Interceptor equilibrium equation:**
  \[
  F_{REk} = Y_k \ast (F_{SRi,REk} + F_{SRe,REk}) \quad \forall k
  \]

  where, \( Y_k \) is the yield of the interceptor, that is, the ratio of the respective stoichiometric coefficients in the equation.

- **sink inlet mass balance:**
  \[
  F_{SKj} = \sum_i F_{SRi,SKj} + \sum_e F_{SRe,SKj} + \sum_k F_{REGk,SKj} \quad \forall j
  \]

  where, \( F_{SKj} \) is the inlet stream of the sink.

2) objective function

OSI minimum value of all interceptor s in C-H-O symbiosis network is taken as the objective function. As shown in equation 6.

\[
f(x) = \min OSI
\]

5 Case study

There were 12 plants in the EIPs of Guizhou province, including Sodium tripolyphosphate, MAP, DAP, LFP, defluorinated tricalcium phospat, forage-grade calcium hydrogen phospha, sodium hexametaphosphate, calcium superphosphate, formic acid, formamide, sodium formate, oxalat. Sources and sinks were identified based on the analysis of details of the products[1]. No.1-No.8 were sources, No.9-No.12 were sinks.

Two solutions were shown in Fig.3. Without i-safe index as the objective function, there were numerous solutions in theory. One of them was shown in Fig.3(a), which included 3 interceptor. It was Carbon dioxide methanation, Carbon dioxide synthesis of methanol and Methane steam reforming, the average OSI is equal to 21.33.
The relevant data of the EIPs were taken into formula (1) - (6), and the NLP optimization model with the minimum average safety index of OSI of the interceptor was established. LINGO was used to solve the optimization model. The units in Fig.3 are kmol/h. The results show that the optimized interceptor network consists of only three interceptors: water gas shift, methane dry reforming unit and carbon dioxide methanol synthesis unit. The average OSI=19 of the obtained intercept network is shown in Fig.3(b). Compared with the interceptor network OSI=21.33 without safety optimization design, the safety index value is reduced because the methane steam reforming unit is replaced by the water gas conversion unit. It is proved that compared with [1], the optimization results show that in the EIPs, 329kmol/h CO2 and 419kmol/h H2O were originally discharged as...
wastes, are converted into sink raw materials by interceptor network. The endogenous 4kmol/hCO was directly used as the raw material for the formic acid plant. EIPs purchased 312kmol/hCH4, 82kmol/hCO2, and 517kmol/hH2O from the cut-off network. As the intercept network transformed CO2, CO2 emissions decreased from 115808t/a before optimization to 0, reducing the greenhouse effect. The water gas shift unit is used, the security is better than the methane steam reforming unit. The number of variables and the constraint equation of the model are greatly reduced, and the calculation time is shortened, which is suitable for large-scale computing problems. It is effective to obtain good security in the early stage of process design.

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References
1. M.M.B. Noureldin, M.M.El-Halwagi Alche. J., 61, 4(2015).
2. D.J. Roddy, Appl Therm Eng, 53(2013).
3. J. Lee, C. Chen, C. Lin, and D.C.Y. Foo, Chem. Eng. Res. Des., 92 (2014).
4. D.C. López-Díaz, L.F. Lira-Barragán, E. Rubio-Castro, J.M. Ponce-Ortega, and M.M. El-Halwagi, Acs Sustain Chem Eng, 3(2015).
5. L.P.E.M. Alnouri S., Comput Chem Eng, 91(2016).
6. S.Y. Alnouri, P. Linke, and M. El Halwagi, Aiche Journal, 60(2014).
7. A.T. Ubando, A.B. Culaba, K.B. Aviso, R.R. Tan, J.L. Cuello, D.K.S. Ng, and M.M. El-Halwagi, J Clean Prod, 136(2016).
8. R.T.L. Ng, D.K.S. Ng, and R.R. Tan, Ind Eng Chem Res, 52(2013).
9. C. Deng, Y. Zhou, W. Jiang, and X. Feng, Int J Hydrogen Energ, 42(2017).
10. M.M. El-Halwagi, Process Integration and Optimization for Sustainability, 1, 3(2017).