MULTIOBJECTIVE PROCESS OPTIMISATION BY APPLYING CONFLICT-BASED APPROACH

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Abstract

This paper proposes a two-stage strategy to deal with multi-objective conflicts in the process synthesis and operation. This approach is founded on the combination of the conflict-based analysis and multi-objective optimization technique. First, a contradiction matrix is formulated to identify the conflicts among the design objectives and next to select the useful heuristics for removing those conflicts. This approach is used for screening and evaluation of the process alternatives in order to generate the efficient superstructure and the useful information for process operation. In the second stage, the multi-objective optimization is carried out by the simulated annealing algorithm (SA) using process simulator ASPEN PLUS. SA algorithm is modified by the dynamically adjusted stepsize (DAS) for continuous variables under the consideration of their importance for the optimization target. DAS speeds up the solution search through adapting the changed stepsize to the current iteration. The proposed approach is illustrated by a case study of the hydrodealkylation of toluene (HDA) process, taking into account process economics and its potential environmental impact.

Keywords

Multi-objective optimization, Conflict-based, Simulated annealing, Dynamically adjusted stepsize

Introduction

The industrial processes have to be designed and operated in a manner enabling the simultaneous fulfillment of the economic criteria, safety, environmental requirements as well as other objectives. The major challenge of design and operation lies in resolving the conflicts between those objectives (Miettinen, 1999). The conflict occurs when improving one objective results in the deterioration of the other ones. Therefore the essential task for process designers is to develop tools for assisting in the trade-off among those conflicted multi-objectives. In view of this issue, current research puts attention on improving the optimization techniques or exploring the quantitative objective indicators to support the optimization at the stage of the detailed design (Dantus et al., 1999). However, the conflicts among the objectives do occur in the early stage of design and they strongly influence the decision-making process of designers. The handling of the conflicts in the early design stage is the precondition for effective process optimization at the stage of the detailed design. Therefore it is an important issue to develop a strategy to handle the conflicts in the context of the whole design process in order to achieve the real optimal solutions.

This work presents a combined approach for dealing with multi-objective conflicts of the process synthesis and operation in both, early and detailed design stages. A conflict-based analysis of multi-objectives in the early stage is aimed at the screening and evaluation of process alternatives. In the second stage, multi-objective optimization is carried out by the modified simulated annealing algorithm (SA). The illustration of this approach is presented using HDA case study.

The Methodology

Overview

The combined approach deals with the design process in two stages as shown in Figure 1.

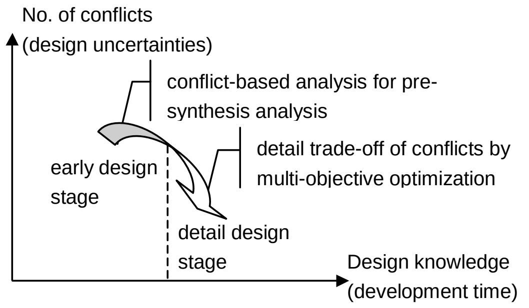

Figure1. The two stage approach

During the early design stage, there is a high possibility that there will occur conflicts among the objectives. It is due to the fact that at early design stage there are the complex design uncertainties as well as the huge decision space. The synthesis task is to remove or decrease the occurrence of the conflicts through the proper decision-making process. A contradiction matrix is proposed as a tool for conflict-based analysis of the synthesis process. In the second stage, multi-objective optimization is realized to trade off the conflicts of objectives. SA algorithm together with ASPEN simulator is used for conducting the optimization. SA algorithm is modified by applying the dynamically changed stepsize of the continuous variables in every iteration.

Modification of Solution Space

TRIZ is an approach to identify the system's conflicts and contradictions for solving the inventive problems (Altshuller, 1998). The main idea of TRIZ consists in the modification of the technical system by overcoming its internal contradictions. Therefore, it is an efficient method for modifying the solution space and early screening the alternatives by the conflict-based analysis.

The formulated contradiction matrix is composed of 8 design objectives, such as economic criteria, product quality, safety, environmental impact etc. The design objectives form the rows and columns of the matrix. 86 design heuristics P_k, k= 1-86 extracted from the available literature (Douglas, 1988 and Smith, 1995) constitute the matrix elements. If the design heuristics P_k influences the objectives i and j, then it is positioned at the intersection of the row i and column j (see Table 1). Every heuristics is characterized by so-called influence coefficient I_i, i=1- 4 and flowsheet phenomena indicator S_j, j= 1-6. The influence coefficient I_i represents the character of the influence on the two concerned objectives when applying the heuristics. The flowsheet phenomena correspond to the region of the flowsheet structure in which the given heuristics should be applied (Li et al., 2002).

The matrix reorganizes the available design heuristics based on their possible influence on the design objectives. It is used for identifying the conflicts among the objectives and handling them by selecting the suitable heuristics considering the concerned objectives. As a result, the design alternatives are screened and preselected to generate the efficient superstructure and useful information for process operation.

Table 1. A fragment of the contradiction table

	1.captial cost	2.operation cost	3.product quality	4.environ. impact	…	8.controll a-bility
1	**	p2 (1, s1) ...	p1(1,s3) ...	P4(1,s6) ...	…	p7(1, s2) ...
2		**	p4(2,s6) ...	p4(4,s6) ...	…	p13(3,s3) ...

Multi-objective Optimization

In this work, multi-objective optimization takes into account the trade-off of the conflicts between the economic criteria and environmental impact. The first objective seeks to minimize the negative profit (-P). The evaluation of environmental impact is based on the waste reduction (WAR) algorithm (Cabezas et al., 1999).

The method of summation of weighted objective functions is used to convert the normalized multi-objectives function into one utility function as shown in Eq. (1), where, $0.0 \le \alpha_i \le 1.0$ and the utility function $u(f_i, \alpha_i)$ is linearly combined with the normalized objective functions and the weighting factors α_i. This method has certain disadvantages. However it can be applied to generate a strongly non-dominant solution that can provide the initial answers for a trade-off among the various objectives (Coello, 2000).

$$\min U(f_i, \alpha_i) = \sum_{i=1}^{n} \alpha_i \frac{f_i(x) - f_{\min}}{f_{\max} - f_{\min}} \qquad s.t. \quad \sum_{i=1}^{n} \alpha_i = 1.0 \quad (1)$$

Potential Environmental Impact

The potential environmental impact (PEI) is proposed by Cabezas et al. (1999) to provide the quantitative indicators that represent the environmental benignity. There are nine different impact categories of PEI, such as the four local toxicological categories: human toxicity potential by ingestion (HTPI), human toxicity potential by dermal, inhalation and exposure (HTPE), aquatic toxicity potential (ATP) and terrestrial toxicity potential (TTP). The relative weight factors of different PEI are customized for specific or local conditions. Here we use the PEI generation per mass of product as the environmental impact criteria. The lower the value the more environmentally friendly the process. It can be calculated based on process data, such as stream flow rates, stream compositions, and environmental impact parameters (Cabezas et al., 1999). The stream flow data can be obtained through the use of a process simulator.

The Modified Simulated Annealing Algorithm

Simulated annealing is a Monte-Carlo technique for multivariable optimization, which has been successfully used to solve many combinatorial problems. The method is based on an analogy to the physical process of annealing (Kirkpatrick et al., 1983). The main advantage arises that there is no assumptions in the form of objective function and constraints. Much work has been done to improve the performance of the SA through modifying the objective function such as the stochastic annealing algorithm (Chaudhuri et al., 1996), and the annealing schedule like $3N^3$ number of movement (Ku et al., 1991). This work focuses on continuous variable optimization via adapting the dynamically changed stepsizes to the current iteration.

Dynamically Adjusted Stepsize

For continuous variables, it is practically impossible to choose the direct neighbors because of the large number of points in the search space. Neither too small nor too large stepsize brings the reasonable solutions. There is always a trade-off between accuracy and robustness in selecting an appropriate step width. The method of step width adaptation (Eq. 2) proved to be able to significantly improve the performance of SA (Nolle et al., 2001). However, the adaptation constant β is empirically designed which limits its applicability and validity.

We observe that β controls the changing speed and the value of the stepsize. For the big values of β, the stepsize is changing fast with the iteration at the high temperature. As the system is getting cooler, the stepsize is changing slowly and reaching small values near the optimal point. The design and optimization shows, that the different variables have the different influence on the particular optimization objectives. It influences in the obvious way the solution searching process. The variable, with the more important influence to the given optimization objective, is assigned the bigger value of β. While the one with the less important influence to the optimization objective, is assigned the smaller value of β to avoid the redundant search in the solution spaces. Therefore, the different values of β are assigned to the various continuous variables in order to reflect their importance for the optimization targets as shown in Eq. (3). It is the function of the weights α_i as well as the weights w_i. The weights α_i of the normalized design objectives reflect their importance for the utility function. The weights w_i mean the importance of the optimized variables for the concerned objectives. The weights w_i, taking the values from 0 to 10, indicate the degree of importance of the particular variable, from unimportant to extremely important. It is determined based on process analysis of the early stage of synthesis. The values of β take the maximum value of the product of the two kinds of weights, which are adjusted for searching every Pareto point. We called the modified term as the dynamically adjusted stepsize (DAS). It changes the stepsize of the continuous variables with every iteration.

$$s(n) = 2s_o \Big/ \left(1 + e^{(\beta n / n_{\max})}\right) \tag{2}$$

$$\beta = \max(\alpha_i w_i) \tag{3}$$

s_0- initial stepsize s - dynamic stepsize at iteration n
n - current iteration n_{max} - maximum number of iterations
β - adaptation constant α - weights of design objectives
w - weights of the importance of the variables (0-10)

Case Study

The HDA process has been extensively studied by Douglas (1988) with a hierarchical heuristic synthesis approach. The problems presented here consist in the conflict analysis between economic criteria and environmental impact for screening and evaluation of process alternatives; and optimization the alternatives by the modified simulated annealing with process simulator.

The primary and side reactions of the process are:

$$Toluene + H_2 \rightarrow Benzene + CH_4$$

$$2Benzene \Leftrightarrow Diphenyl + H_2$$

The detail process specification refers as Douglas (1988).

Modification of Solution Space

Considering the objectives of profit and environment impact, there are three identified conflicts: among the capital and operating cost (1x2), capital cost, operating cost with environmental impact (1x4, 2x4). Based on the contradiction matrix, the heuristics concerned with those conflicts are analyzed using the value of the influence coefficients. For example, Heuristics 2 suggests using an excess of one of the reactant. Its influence coefficient indicates that raw material efficiency is improved but the capital cost is increased simultaneously. From the point of view of the environmental impact, the heuristics 58 (recycling the by product for inhibiting its formation at the source) proposes recycling diphenyl byproduct instead of its recovery; and the heuristics 79 suggests that there should be vapor recovery system arranged on the purge stream. Then suitable heuristics are selected to screen and evaluate the corresponding alternatives. The compact superstructure can be achieved ensuring the efficient structure interconnection and useful information of operations. Those can reduce the combination size of the problem to assist the next multi-objective optimization. The detail description can be found in Li et al. (2002).

Multi-Objective Optimization

In terms of economics and potential environmental impact, the multi-objective optimization problem in this work is subject to the following constraints: the hydrogen feed has a purity of 95%; the purity of benzene product is at least 95%; one of the objective functions is profit defined as product sold minus raw material costs; the relative weight factors of different environmental impacts are set to 1. The stream cost data and environmental impact index refers as presented in Fu et al. (2000)

The SA algorithm with ASPEN simulator is applied as the optimization techniques. It optimizes the configuration through the evolution of the structural and stream states. However it is very computationally demanding to get the Pareto set for each possible configuration. In order to verify the effect of the modified SA, there are presented the results of optimization of flowsheet composed of adiabatic reactor, and stabilizer separation column and having the diphenyl stream as byproduct. Three continuous variables are optimized with the bounds and initial values listed in Table 2. The weights of importance of three variables are determined as 7, 9, 9 for profit objective and 5, 5, 9 for environmental impact based on process analysis. Calculations are performed on Pentium III running at 700 MHz frequencies.

The obtained Pareto set is plotted in Figure 2 presenting the comparison between the modified SA with DAS and the original SA under the same initial data. The nearly identical results confirm the accuracy of this modified method. The efficiency of the method is measured by the number of the function evaluation and CPU calculation time of every obtained Pareto points as shown in Figure 3. It is proved that, for the run of every Pareto point, the modified SA is more efficient with respect to the convergence and the amount of the computational work. Table 3 shows the optimized results of minimized and maximized objective functions, the corresponding values of continuous variables and the output flowrate of five components.

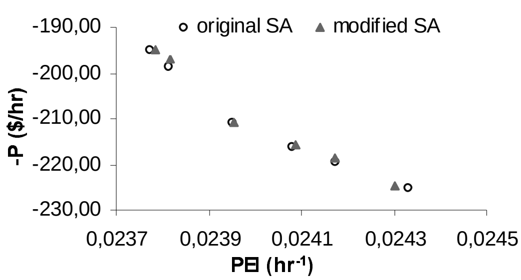

Figure 2. The optimal Pareto set

Table3. Results for the optimized process alternative

	Min P	Max P	Min PEI	Max PEI
Profit ($/hr)	182.71	224.98	195.81	210.87
PEI (10^{-2}/hr)	2.625	2.433	2.382	2.695
Hydrogen feed (kmol/h)	240.00	250.00	240.59	249.89
Toluene feed (kmol/h)	130.00	120.00	129.92	121.88
Conversion	0.600	0.800	0.797	0.601
Output (kg/h)				
Hydrogen	223.42	260.089	223.93	257.18
Methane	2264.44	2120.04	2271.27	2142.71
Toluene	78.255	32.441	34.146	75.622
Diphenyl	1847.15	1722.51	1861.53	1733.36
Benzene	8217.15	7601.14	8233.58	7700.63

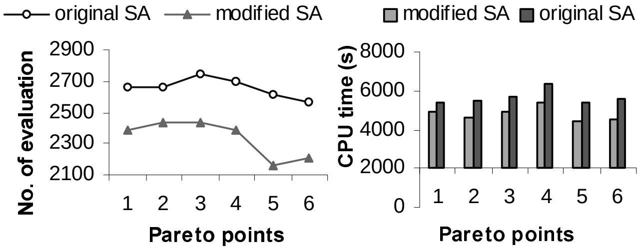

Figure3. The evaluation of optimal points

Table2. The bounds and initial values for variables

Continuous variables	Lower	Upper	Initial value
Hydrogen feed (kmol/h)	240	250	245
Toluene feed (kmol/h)	120	130	125
Conversion of reactor	0.6	0.8	0.7

Conclusions

The paper proposes a two-stage approach to deal with the conflicts resulting from the multi objective nature of the process synthesis and operation. The conflict-based analysis of the objectives is used for screening and evaluation of the alternatives in the early stage of design. It assists to generate the efficient superstructure and useful information for the second stage, multi-objective optimization. The optimization technique is based on the simulated annealing algorithm using process simulator ASPEN PLUS. For optimizing the continuous variables, SA adapts the DAS to current iteration. The optimization results suggest that the proposed method can improve the computational efficiency while keeping optimization accuracy. The proposed approach is illustrated by HDA case study where the economic criteria as well as the environmental impact are set as the optimization criteria. The complete Pareto set over the flowsheet superstructure will be generated in the future work.

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