https://doi.org/10.1016/j.compchemeng.2019.106618

Stakeholder-oriented multi-objective process optimization based on an improved genetic algorithm

Su Yang[ab], Jin Saimeng[ab], Zhang Xiangping[c], Shen Weifeng[ab], Mario R.Eden[d], Ren Jingzheng[e]

[a] School of Chemistry and Chemical Engineering, Chongqing University, Chongqing 400044, China
[b] National-municipal Joint Engineering laboratory for Chemical Process Intensification and Reaction, Chongqing University, Chongqing 400044, China
[c] Beijing Key Laboratory of Ionic Liquids Clean Process, CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China
[d] Department of Chemical Engineering, Auburn University, Auburn, AL 36849, United States
[e] Department of Industrial and Systems Engineering, The Hong Kong Polytechnic University, Hong Kong SAR, China

Abstract

Multi-objective optimization (MOO) is frequently used to solve many practical problems of chemical processes but process designers only need a limited number of valuable solutions in the final results. In this study, an optimization strategy associated with an improved genetic algorithm was developed to search valuable solutions for stakeholders' preference more purposefully. The algorithm was improved to reduce overlapping solutions as a result of the discrete variables in practical problems, and it allowed users to set a reference point or an angle associated with a reference point to make solutions converge into the preferred spaces. Three test functions and two practical problems were used to highlight that the proposed strategy could make designers optimize processes more efficiently. Especially, the angle-based algorithm could be more effective than the distance-based one on the tri-objective problems. Thus, the developed strategy is robust in the optimization of processes assisted with the designer's preference.

Keywords: Multi-objective optimization; Preference; Process optimization; Genetic algorithm

1. Introduction

As the global energy consumption and environmental pollution are dramatically increasing, the improvement of industrial sustainability becomes more and more important. The reduction of energy consumption and waste discharge is a significant purpose of process optimization and product design. In practice, the process optimization or product design problem may involve more than one objective function, or even multiple conflicting objectives. Therefore, many researches have focused on the application of multi-objective evolution algorithms (MOEAs) to solve the MOO problems in industries (e.g. Beykal et al., 2018; Biegler and Grossmann, 2004; Datta et al., 2017; Garcia and You, 2015; Herring Iii and Eden, 2015; Khurana and Farooq, 2019). The advantage of MOEAs is that it can provide a solution set including more than one solution for process designers. It should be noted that the optimization of such problems in chemical engineering has its own characteristics different than in other fields. On one hand, the process designers' experience and knowledge may affect their final choice of solutions and even benefit the efficiency of optimization (Wang et al., 2018). On the other hand, there may be a need to optimize the discrete decision variables with continuous variables for a chemical process simultaneously.

There are many studies focusing on the applications of MOEAs for process optimization or product design. According to the decision-making order, Coello *et al.*(2007) classified the MOEAs into three categories: *a priori*, *interactive* and *a posteriori* techniques. Among them, the *a posteriori* techniques, in which the decision maker (DM) has to make the after choice based on the trade-offs observed in the set, are the most popular strategies in process optimization (Rangaiah, 2009). It is remarkable that the Non-dominant Sorting Genetic Algorithm (NSGA, Srinivas and Deb, 1994) and the improved edition namely NSGA-II (Deb et al., 2002) have been employed to solve many issues of chemical engineering (e.g. Habibi et

al., 2018; He and You, 2015; Muñoz López et al., 2018; Parhi et al., 2019; Yan et al., 2016). In these studies, a number of the current optimization works assume that the DM would be interested in generating the entire *Pareto* set of a problem. Unfortunately, sometimes it is difficult and time-consuming to achieve all *Pareto* solutions in the *a posteriori* techniques. In the worst case, the finally obtained solutions are even far from the true *Pareto* set, since DMs could not foreknow the reasonable search space of variables or do a calculation without enough iterations. To avoid this unexpected possibility, the DMs often extend the search space of a practical problem and then take a longer computational time. However, perhaps only one solution can be adopted according to the DM's preference at last.

In most cases, DMs may have some intuition originated from their experience and knowledge, and may speculate their interesting search spaces (Branke et al., 2001). Therefore, some MOEA researchers (Coello, 2000; Greco et al., 2005) have incorporated the DM's preference into the *a posteriori* techniques to speed up convergence. A new algorithm of the non-dominated sorting called "r-dominance" is introduced by Said *et al.* (2010), which has the ability to sort *Pareto*-equivalent individuals based on the DM's preference. Xie et al. (2012) introduced an angle based dominance (A-dominance) relation for incorporating the DM's preferences. Moreover, the *interactive* algorithms allow the DMs to adjust the optimization parameters while observing the changes in the solution set. More recently, some novel interactive strategies have been proposed to introduce the DM's preferences for the higher efficiency. Bortz et al. (2014) proposed an efficient MOO strategy that allowed DMs to introduce and update their preferences interactively with a visual optimization tool. In such a case, the lower computational expenses are achieved because two scalarizations were combined to approximate the Pareto set and did not treat the process simulator as a black box.

Vallerio et al. (2015) proposed an interactive method based on geometric considerations to reduce the possibility that the extreme part of the Pareto set is overlooked. In this method, the DMs can actively choose the preferred part of the Pareto set to investigate. These interactive methods can introduce the DM's preference in real-time at a low computational cost, which are highly significant to the dynamic process optimization. However, most process designers often pick out the preferred solutions in the final solution set rather than introduce their preferences into the optimization process using these algorithms.

On the other hand, as the existing MOEAs often have mechanisms of diversity preservation, many overlapping solutions are not likely to exist in each population when they are applied to MOO problems with continuous decision variables and/or many objectives (Ishibuchi et al., 2005). Although all these algorithms had been validated on the non-constraint and continuous issues, they could show the low efficiency of optimization on the MOO problems involving discrete decision variables as the result of overlapping solutions (Ishibuchi et al., 2005; Wang et al., 2015). To some extent, all these studies are useful for the process or product designers to obtain the optimum solutions. However, the discrete variables and the preferred solution selection can hardly be avoided in the problems of chemical engineering, thus it is significant to improve the strategies and algorithms of MOO for chemical process.

To solve the above-mentioned problems and inspired by the interactive methods, we developed a strategy that enables designers to optimize a process more purposefully and efficiently. The proposed method involves the application of a sensitivity analysis (SA) to formulate the reasonable search space, and an improved edition of NSGA-II from two aspects: the introduction of a designer's preference and the detection/deduplication of overlapping solutions. Two preference-based algorithms, r-dominance and A-dominance, were employed

to guide the convergence direction of solutions, while a mechanism checking and reducing overlapping solutions is proposed to improve the quality and efficiency of convergence. A workflow of the proposed strategy assisted with the improved algorithm is introduced and the details of the improved NSGA-II is also disclosed. Three case studies were employed to validate the strategy with the improved algorithm from two insights: the mathematical sense and the practical application on chemical processes. Hereinto, the benefits brought by the designer's preference and the improved algorithm were discussed. In the first case study, three test functions are adopted to examine the improved NSGA-II. Afterwards, a case of the extractive distillation is employed to confirm the advantages of the proposed strategy compared to the original NSGA-II. Another more complex process is exemplified to validate the effectiveness of preference-based algorithm on tri-objective problem. The results of these case studies show the performance difference between r-dominance and A-dominance, and the reduction of overlapping solutions. Finally, the more efficient optimization is obtained by the improved algorithm. For ease of applying the proposed strategy, a MOO tool involved the improved NSGA-II is developed, in which a mechanism for error monitoring is also introduced.

2. The strategy of MOO with the designer's preference

The process or product designers as the representative of the stakeholders/decision-makers usually have different preferences on these optimization objectives. The search space of optimization model involving the constraints of design or operational variables was usually determined intuitively in the previous MOO problems. The SA could help designers to understand the relationships among objectives and variables, even pick out the optimal solutions (Yang et al., 2019b). As such, it is recommended that a SA should be implemented to formulate the MOO problem more reasonably. In this work, a strategy combining the improved

NSGA-II with the SA was proposed to make the optimization more purposeful.

In general, the optimization with the strategy can be divided into three stages (as presented in **Fig. 1**), and they are:

(1) building the process model in the process simulator which should be converged on several initial parameters;

(2) identifying the key operating and design variables for the less blindness of optimization, and the designers can find the rough search space through observing the changes of some important indicators using sensitivity analysis (SA);

(3) establishing a MOO problem with reasonable constraints based on the SA results, where the designers as the DMs can introduce the preference settings (*e.g.* a reference point, objective weights and the threshold) according to their own knowledge and experience. Finally, the non-dominated solutions with a DM's preference can be achieved when running hundreds of iterations.

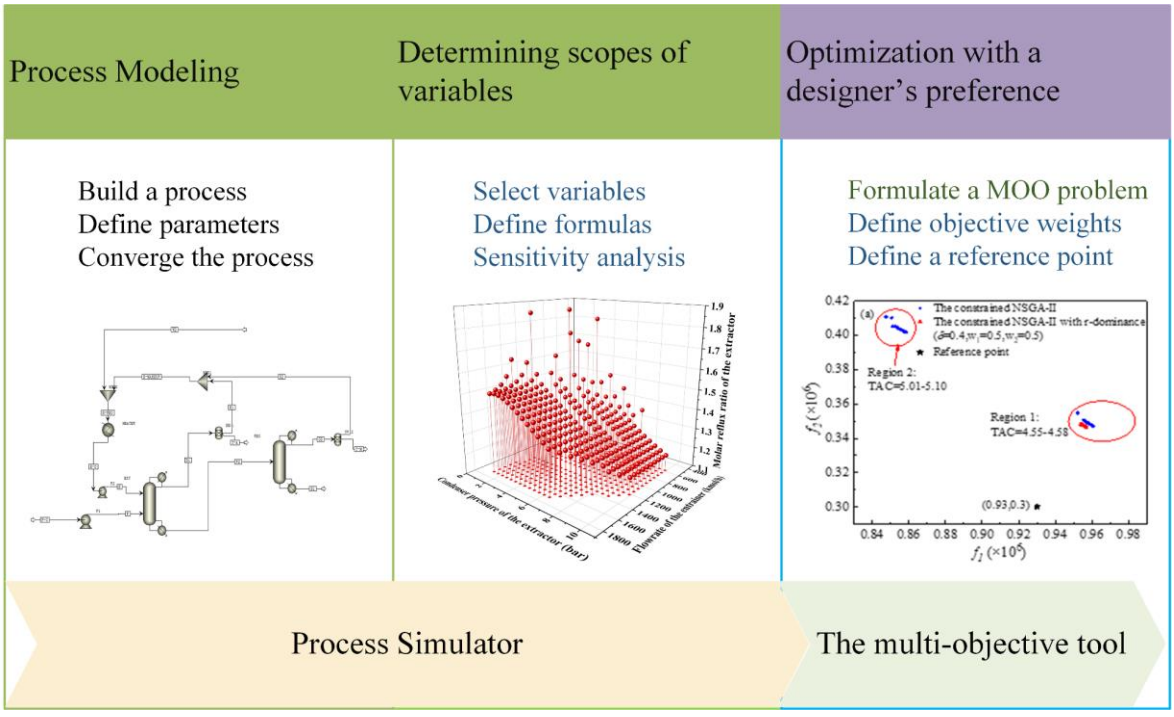

Fig. 1. The workflow of the proposed strategy for multi-objective optimization with a designer's preference.

Within the strategy, a process simulator was used to build process models and carry out the SA, while the improved NSGA-II was enhanced by improving non-dominated sorting and inhabiting overlapping solutions.

2.1. Mathematical formulation

A multi-objective model which aims to simultaneously maximize/minimize two or more conflicting objectives with several decision variables and constraints can be firstly defined, as presented in Eq. (1a) - (1d):

$$\text{Maximize/Minimize} \quad f_1(\boldsymbol{x}) \quad f_2(\boldsymbol{x}) \quad \cdots f_N(\boldsymbol{x}) \tag{1a}$$

Subject to:

$$\boldsymbol{x}^L \leq \boldsymbol{x} \leq \boldsymbol{x}^U \tag{1b}$$

$$h(\boldsymbol{x}) = 0 \tag{1c}$$

$$g(\boldsymbol{x}) \leq 0 \tag{1d}$$

where, decision variables can be either continuous or discrete with a lower and upper constraints ($\boldsymbol{x}^L$ and $\boldsymbol{x}^U$) explicitly. Other constraints presented by equalities or inequalities implicitly ($h(x)$ and $g(x)$) can be determined in the process models commonly. The number of equalities and inequalities constraints can be zero, a few or a lot depending on the specific problem. For the MOO of a certain process, the equalities, such as the balance of mass and energy, are easily formulated and determined in process simulators. In contrast, it is usually difficult to formulate the inequalities (e.g. the requirement of product purity) in a process simulator directly. As such, the inequalities are often converted to an equality with the design specification in a simulator. Despite this conversion is effective in most cases, it narrows the search spaces of decision variables and objectives. Another way (Segovia-Hernández and Gómez-Castro, 2017) penalizing the solutions outside the constraints is implemented when the

objective functions are calculated. It is easy to realize the penalization method within the external solver such as the optimization toolbox in MATLAB®, but the constraint-handling method of the specific MOEA will not work.

On the other hand, the formulation of a MOO problem is also related to the preferences, knowledge and experience of designers who often defines intuitively a decision space at the initial stage of optimization. Nevertheless, it might be blind to choose the decision space subjectively, which could result in some problems. For example, the solutions are still unsatisfying or impracticable when the boundaries of decision variables are reached. To reduce the uncertainty caused by the subjectivity, the SA is applied in the proposed strategy for the formulation of MOO problems. Although the reasonable search space is helpful to achieve a whole *Pareto*-optimal set of solutions, the designers' preference cannot be easily considered at the model formulation of a practical issue. Hence, the improved NSGA-II with the modified non-dominant sorting was introduced into the strategy.

2.2. The constrained NSGA-II with the user's preference

In the original edition of the constrained NSGA-II, a procedure of binary tournament selection was used to compare two random individuals in the population and then choose the optimal individual to fill the mating pool. Generally, there may be at most three possibilities for the two individuals: 1) both individuals are feasible; 2) one is feasible and the other is not; and 3) both are infeasible. The criteria of feasible individuals in the MOO problem were summarized in **Table 1**. In detail, the dominant relationships between them were as follows:

(1) If one individual is feasible while the other is not feasible, the feasible one will be chosen;

(2) Once both are infeasible, the individual with smaller overall constraint violation will

be selected; and

(3) When both two individuals are feasible, the better one will be picked out. In short, the selected individual dominates the other one.

Table 1 The feasible criteria of individuals for different constraints

Constraints	Content	Feasible criteria	Setting position
Equalities	Mass and energy balance Other balance equalities	The process model in simulators is converged	simulator
	User-specified equalities	The tolerance values are smaller than the specified ones	simulator
Inequalities	User-specified inequalities	The values of variables are within lower and upper bounds	MOO solver

Obviously, there are not any preferences of DMs considered in the binary tournament selection of the constrained NSGA-II. Hence, two preference-based dominant relationships (*i.e.* r-dominance (Said and Bechikh, 2010) and A-dominance (Xie et al., 2012)) were employed to modify the dominant relationships as illustrated in **Fig. 2**. Unlike *a priori* techniques, these two algorithms sort a *Pareto* non-dominated set in obedience to a strict partial order instead of relying on the aggregation functions.

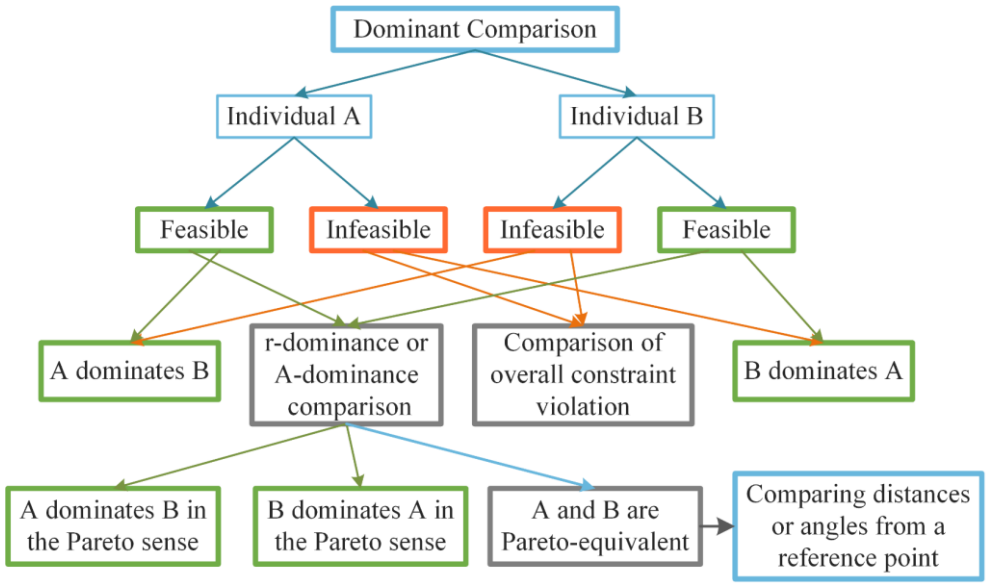

Fig. 2. A classification of dominant comparison between two individuals in non-dominated sorting.

r-dominance algorithm

The preferred solutions are closer to the reference point with the weighted Euclidean distance calculated by Eq. (2d) in the algorithm. When the constrained NSGA-II is combined with r-dominance (Said and Bechikh, 2010), the definition of domination between two individuals *A* and *B* is presented as below.

Definition 1: Assuming a population of individuals ***P***, a reference point ***r***, and a weight vector ***w***, an individual *A* is said to dominate an individual *B* (denoted by $A \prec B$, the "$\prec$" is a dominant comparison operator) if one of the following statements holds true (Said and Bechikh, 2010):

(1) *A* and *B* are both feasible:

a) *A* dominates *B* in the *Pareto* sense;

b) *A* and *B* are *Pareto*-equivalent and $D(A, B, \boldsymbol{r}) < -\delta$, where $\delta \in [0, 1]$ and

$$D(A,B,\boldsymbol{r}) = \frac{Dist(A,\boldsymbol{r}) - Dist(B,\boldsymbol{r})}{Dist_{\max} - Dist_{min}} \tag{2a}$$

$$Dist_{\max} = Max_{z \in P} Dist(z,\boldsymbol{r}) \tag{2b}$$

$$Dist_{\min} = Min_{z \in P} Dist(z, \boldsymbol{r}) \quad (2c)$$

$$Dist(A, \boldsymbol{r}) = \sqrt{\sum_{i=1}^{M} w_i \left(\frac{f_i(A) - f_i(\boldsymbol{r})}{f_i^{\max} - f_i^{\min}} \right)^2}, w_i \in [0,1], \sum_{i=1}^{M} w_i = 1.0 \quad (2d)$$

δ is termed the non-r-dominance threshold.

(2) A is a feasible solution but B is infeasible.

(3) A and B are both infeasible:

a) A has a smaller overall constraint violation.

b) A has an equivalent overall constraint violation to B *while* A has the better fitness values.

A-dominance algorithm

The algorithm is angle-based binary tournament that adopts the angle $\alpha \in [0, \pi/2]$ control the preferred region near a reference point $\boldsymbol{r}$ (see Fig. S1 in the Supporting Information). The related definitions of A-dominance (Xie et al., 2012) are shown as follows:

Definition 2 (Ideal Point): One individual $X \in \boldsymbol{P}$, the ideal point $\boldsymbol{b}$ is defined as b_i = Min($f_i(\boldsymbol{x})$), $\forall f(\boldsymbol{x}) \in$ *Pareto* front, where the symbol $\boldsymbol{x}$ means the vector of decision variables for an individual X.

Definition 3 (Near Point): The near point $\boldsymbol{g}$ is defined as:

$\boldsymbol{g} = \{g | \forall\, h \in \boldsymbol{P}, Dist(g, \boldsymbol{r}) < Dist(h, \boldsymbol{r})\}$, where $\boldsymbol{r}$ is the reference point, h is a set of points near the reference point $\boldsymbol{r}$. The symbol $\boldsymbol{g}$ refers to a set of points including a point g that has the shortest distance from the reference point $\boldsymbol{r}$.

Definition 4 (Individual Angle): Any two individuals X, $Y \in \boldsymbol{P}$, Angle(X, Y) = acos $((\boldsymbol{i}*\boldsymbol{j})/(|\boldsymbol{i}|*|\boldsymbol{j}|))$. Where

$$\boldsymbol{i} = ((x_1 - b_1)/(f_1^{\max} - f_1^{\min}), \ldots, (x_i - b_i)/(f_i^{\max} - f_i^{\min}), \ldots, (x_m - b_m)/(f_m^{\max} - f_m^{\min})) \quad (3a)$$

$$\boldsymbol{j} = ((y_1 - b_1)/(f_1^{\max} - f_1^{\min}), \ldots, (y_i - b_i)/(f_i^{\max} - f_i^{\min}), \ldots, (y_m - b_m)/(f_m^{\max} - f_m^{\min})) \quad (3b)$$

The f_i represents the i-th fitness function while the b_i is the theoretical optimal value of i-

th fitness function. Meanwhile, the superscript "max" indicates the maximum value of f_i in the current population, and the superscript "min" means the minimum value of f_i.

Definition 5 (A-dominance):

Any two individuals X, $Y \in \boldsymbol{P}$, X is said to A-dominate Y (denoted by $X \prec Y$) if and only if one of the following statements holds true:

(1) X and Y are both feasible:

a) X dominates Y in the *Pareto* sense.

b) X and Y are Pareto-equivalent and Angle $(Y, \boldsymbol{g})$ − Angle $(X, \boldsymbol{g}) > \alpha$, where $\alpha \in [0, \pi/2]$.

(2) X is a feasible solution but Y is infeasible.

(3) X and Y are both infeasible:

a) X has a smaller overall constraint violation.

b) X has an equivalent overall constraint violation to Y, but X has the better fitness values.

The two algorithms, r-dominance and A-dominance, integrating the DM's preferences cause the partial selection pressure "stronger" than the *Pareto* dominance one. Additionally, the modifications in the non-domination principle do not change the computational complexity of NSGA-II. The rest of NSGA-II implementations as described earlier can be utilized as usual.

2.3. Reducing the overlapping solutions

As mentioned before, the overlapping individuals may exist in the evolution populations because the MOO problems in chemical engineering often include discrete variables. Intuitively, the unaccepted and redundant solutions may waste the time of optimization and debase the availability of the solution set for making a decision (Zhu et al., 2009). Before the introduction of the following algorithm, the definition of the overlapping individuals is shown as:

Definition 6 (overlapping individuals):

Any two individuals X, $Y \in \boldsymbol{P}$, the symbols, $\boldsymbol{x}$ and $\boldsymbol{y}$, are defined as the decision variables of X and Y respectively. The f_i represents the i-th fitness function. An individual X is said to overlap another individual Y if and only if one of the following statements holds true:

(1) The values of all decision variables are equal ($x_1=y_1$, $x_2=y_2$, …, $x_i=y_i$).

(2) The values of all objective functions are equal ($f_1(\boldsymbol{x})=f_1(\boldsymbol{y})$, $f_2(\boldsymbol{x})=f_2(\boldsymbol{y})$, …, $f_i(\boldsymbol{x})=f_i(\boldsymbol{y})$).

Notably if two individuals have the identical values of objective function, it is possible that they have different values of decision variables. In other words, the two individuals are considered as two overlapping individuals but not the exactly same individuals in this study. The mechanism for reducing the number of redundant solutions as shown in **Fig. 3** includes two operations to improve the constrained NSGA-II: one is to deduplicate the overlapping individuals from the merged population, and another one refers to extra mutation for suppressing the generation of individuals with the same decision variables. In the first operations, duplicate copies of individuals were removed in the decision and objective spaces before the non-dominant sorting. After the non-dominant sorting was finished, two individuals were randomly sampled as parents from the optimal solution set and then used to reproduce two children using crossover or mutation. However, there is a possibility to generate two identical children in the variable space, thus the extra mutation based on the normal distribution is used to bring small variations in the chromosome of one child. As the varied variables are still kept around the original variable values of parent, the second operation are named “weak mutation” that aims to ensure that the overall search direction is not changed substantially. In addition, the strength of the weak mutation can be adjusted by two parameters: the standard deviation σ controlling the dispersion of a chromosome, and the sampling number N_s describing

the number of random data points sampled from the normal distribution. If the weak mutation is activated, each chromosome of a child will be assigned one new value from a list of N_s values randomly. The new value is the closest one to the original value of a decision variable. It is noted that the crossover and mutation of the original NSGA-II are still remained in the improved edition. In this work, the simulated binary crossover (SBX) (Deb et al., 2002) was employed as the crossover operator while the polynomial mutation is used as the main mutation.

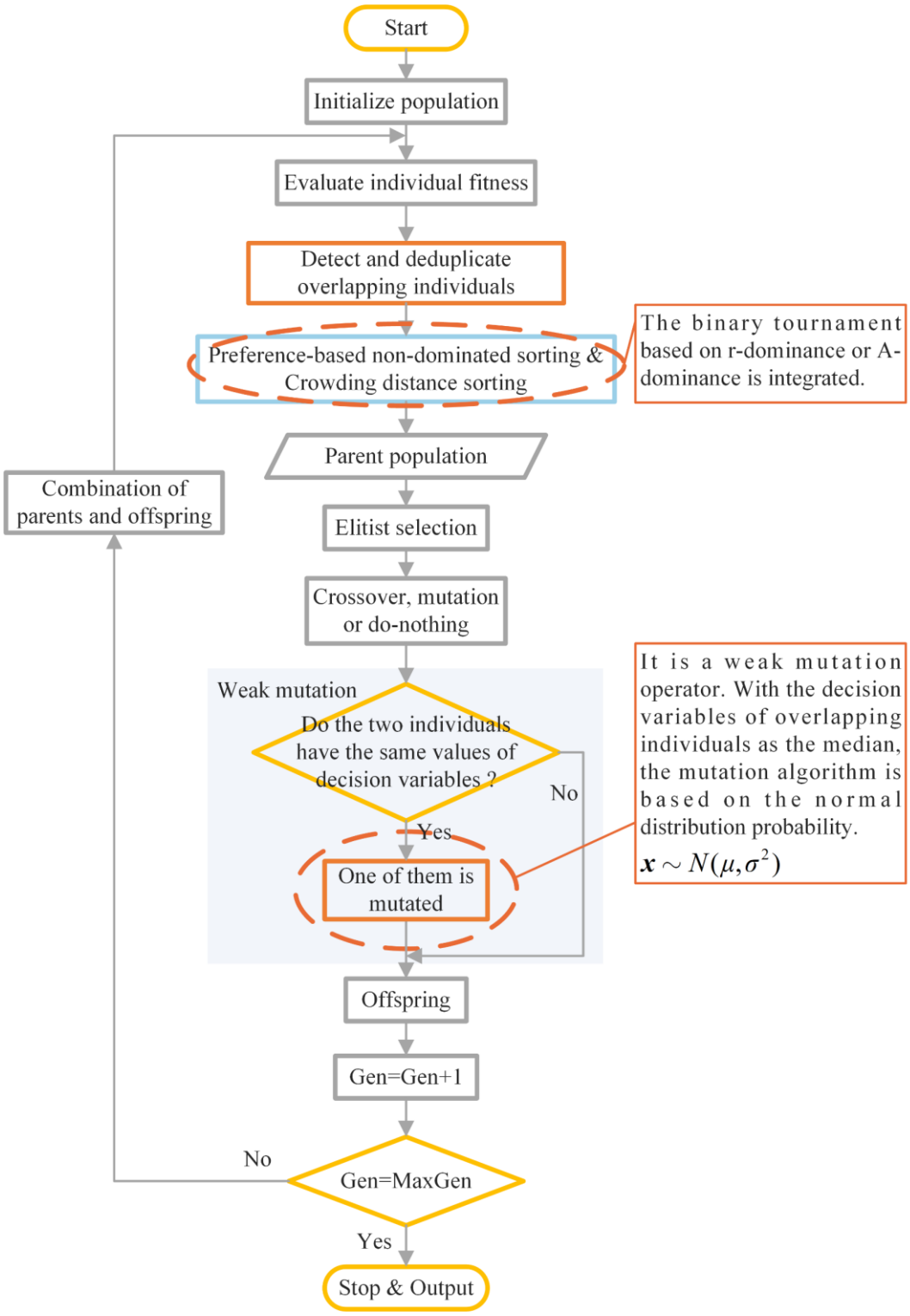

Fig. 3. The flowchart of the improved NSGA-II.

3. The multi-objective optimization system

A system named NAS214 with the improved NSGA-II was developed to applied as a solver in the proposed strategy. Several parameters representing the user's preference such as

the reference point, threshold and objective weights can be defined in the developed tool. The architecture of the system shown in **Fig. 4** includes three parts: a graphic user interface (GUI), a process simulator and MOEAs. Among them, the process simulator is considered as an opaque operator similar to the black box which is only responsible for calculating a process model. Herein, Aspen Plus® was employed as the process simulator providing a node tree for accessing the internal variables and some modules (e.g. unit operations, calculators and design specifications) to calculate the values of user-defined equalities and inequalities.

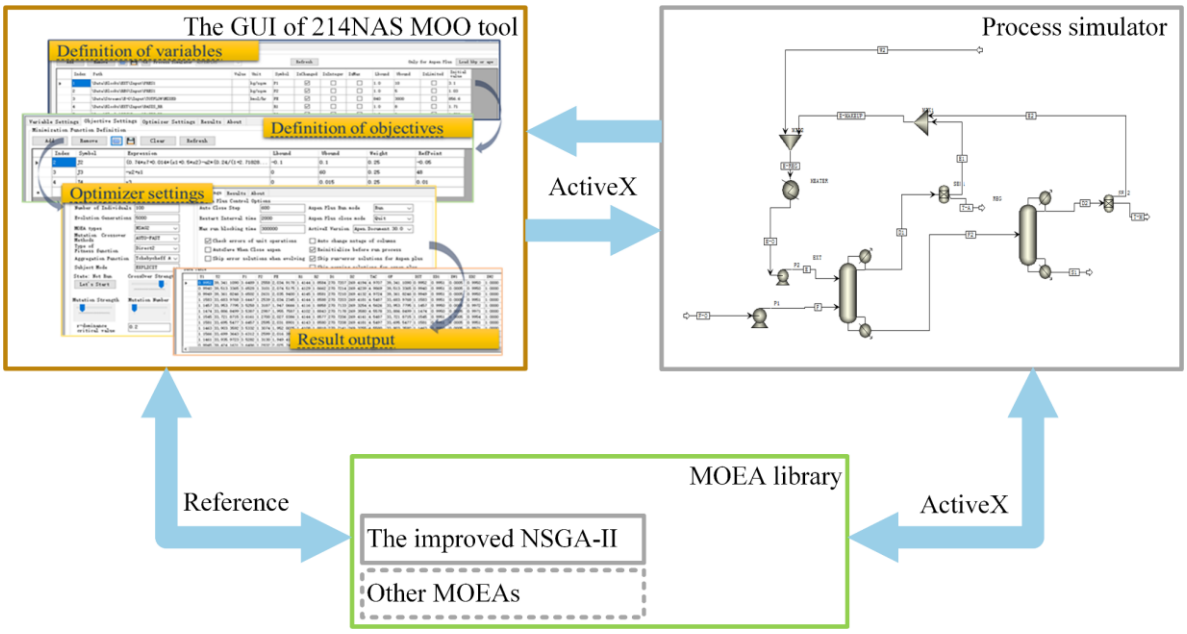

Fig. 4. The scheme of the NAS214 tool for multi-objective optimization

In the MOO of a chemical process, the MOEAs repeatedly call the process simulator. However, there exists some possibilities that the process simulator crashes occasionally causing the optimization to be interrupted. As such, A wrapper for controlling and monitoring the process simulator was implemented in the program, which includes a mechanism presented in **Fig. 5** to maintain the uninterrupted operation of simulators.

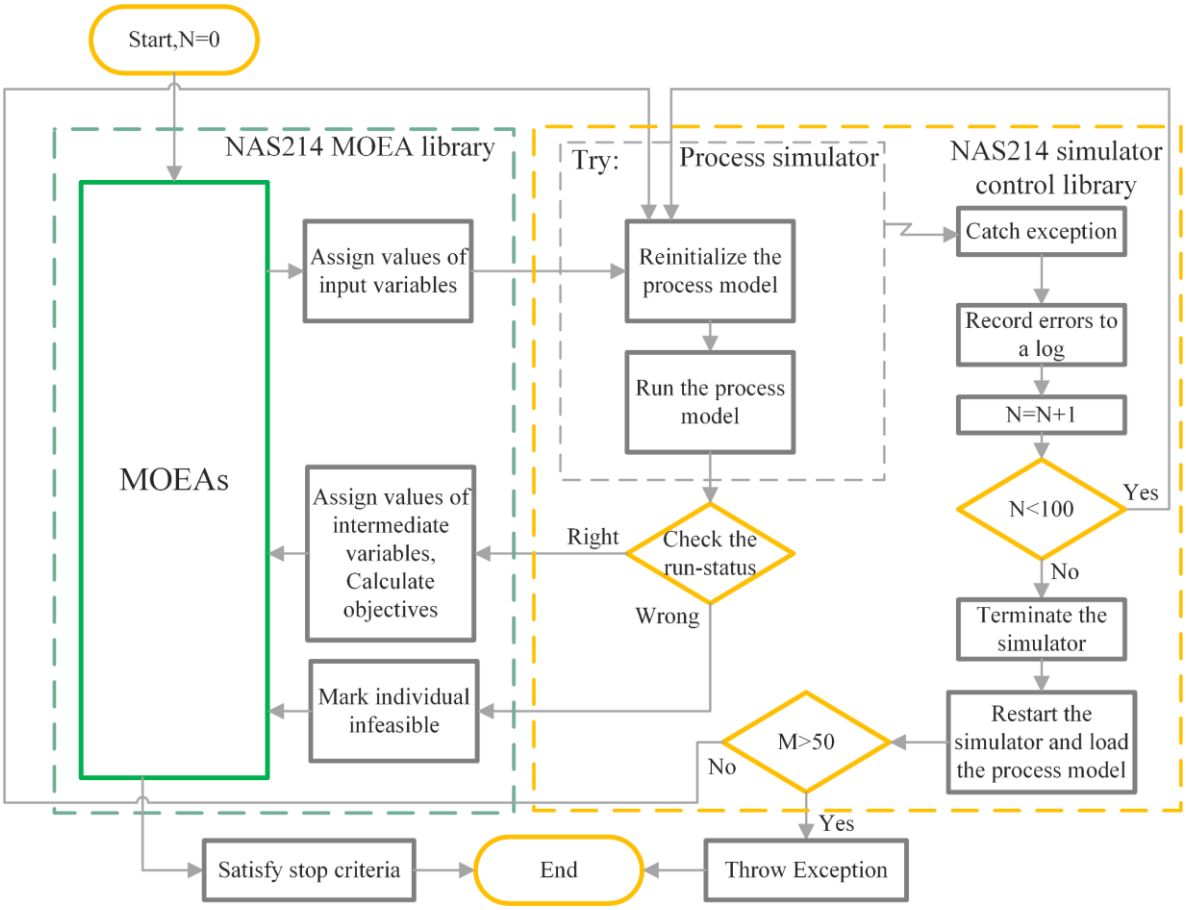

Fig. 5. The procedure of monitoring and controlling the simulator in the NAS214 MOO tool.

In the mechanism, a try-block was used to detect the runtime error during the calculation. When no errors happen in the try-block, the results were checked by the process simulator and then the right one is passed to MOEAs. If an exception occurs inside a try-block, any remaining code in the same try-block will not be executed. The right of control is immediately transferred to the outer catch-block, a logger will record the exception and a counter will increase one. Subsequently, if the value of the counter N is less than a pre-defined threshold (*e.g.* one hundred as depicted in **Fig. 5**), the procedure will run the try-block again. But if N is greater than the threshold, the program will shut down the current simulator instance and restart a new one. Another counter M records the restarting times of the simulator, the try-block will be executed again if M is less than the threshold. With the help of the whole mechanism, the developed program can run an optimization task for a long time unattended.

4. Case studies

Several test functions were utilized to evaluate the effectiveness of the improved algorithm mathematically in section 4.1. In order to illustrate the developed model, two illustrative cases were studied. The first example illustrated in section 4.2 was the extractive distillation involving two objectives. The second example in section 4.3 refers to a process of methanol synthesis which is a tri-objective optimization problem, and it was selected to evaluate the improved algorithm with the different preference-based dominant rules. Incidentally, all case studies run with the developed tool on a desktop computer (Intel i5-8400 @ 3.8GHz).

4.1. **Case 1:** Test functions

This case was employed to verify the improved NSGA-II with a DM's preference from a mathematical perspective. The first test function, ZDT3 (Deb, 2011), was utilized to demonstrate the availability of the NSGA-II with r-dominance or A-dominance on the unconstrained MOO problem with different reference points. Subsequently, two constrained test functions similar to the constrained MOO problems commonly encountered in chemical processes, BK (Binh and Korn, 1997) and CH (Chankong and Y. Haimes, 1983) problems, were applied to verify the improved NSGA-II. The objective weight vectors of the ZDT3 and BK problems were both set to (0.5, 0.5). After 200 generations with the 100 individuals are iterated, the solution sets were achieved as shown in **Fig. 6-8**. When the r-dominance algorithm was activated, the solutions converge into a smaller range based on the position of a reference point. Moreover, it can be observed that the parameter δ controls the dispersion of preferred solutions in r-dominance while the parameter α plays the same part in A-dominance (see **Fig. 7**). As shown in **Fig. 8**, a bias on the distribution of the preferred solutions is caused by adjusting the weight of each objective. As a result, designers can adjust the coordinate of a reference

point, objective weights and the threshold δ to control the position and distribution of solutions in r-dominance. Likewise, using the A-dominance algorithm, users can change the parameter α and the position of a reference point to control the distribution and position of solutions.

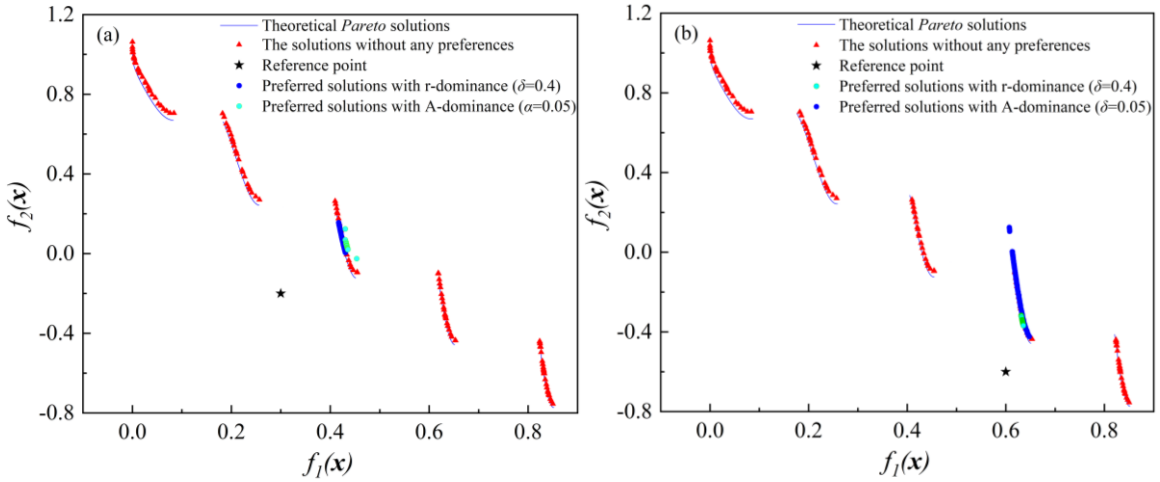

Fig. 6. The effect of different reference points on the two-objective ZDT3 problem

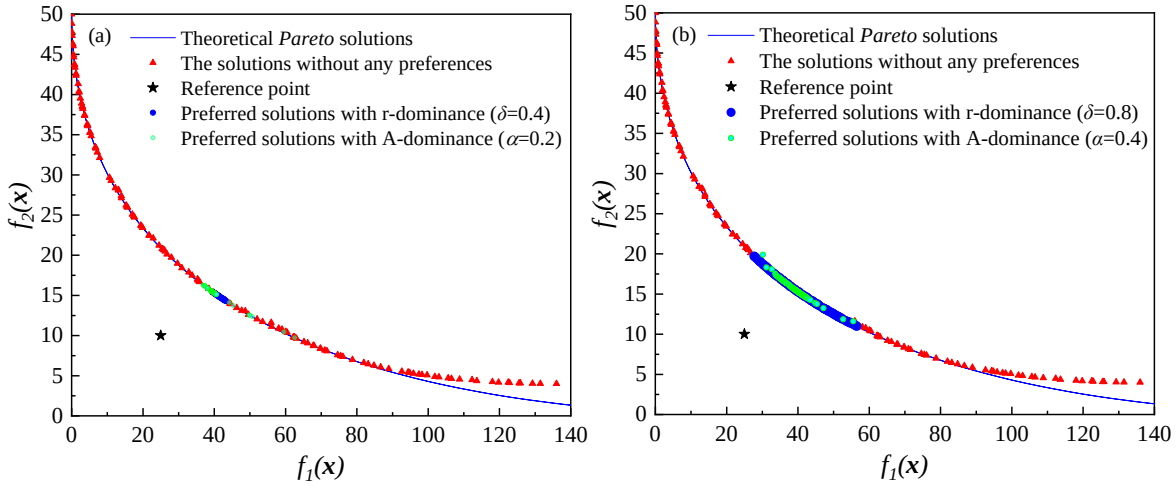

Fig. 7. The effect of different threshold parameters on the two-objective BK problem.

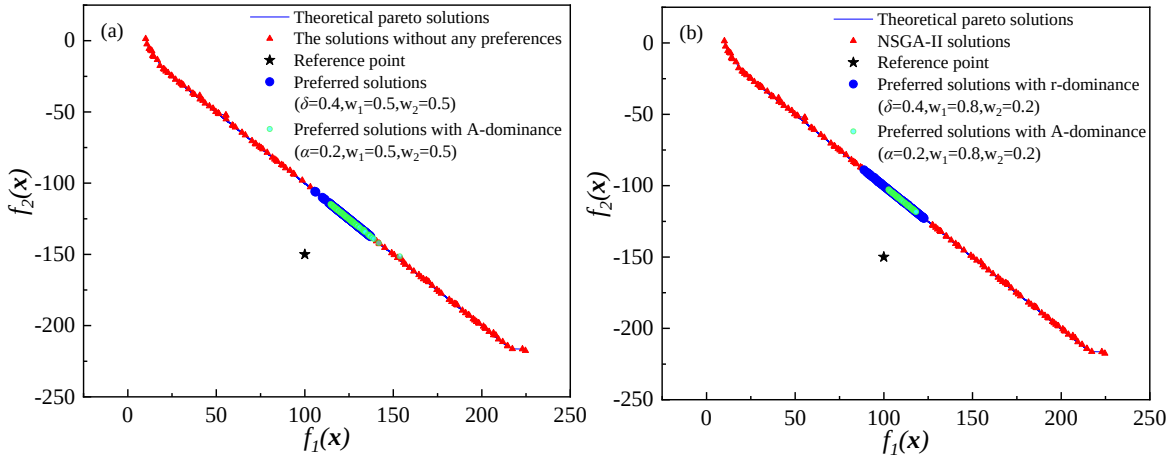

Fig. 8. The effect of different weight vectors on the two-objective CH problem.

Furthermore, the mechanism of reducing the overlapping solutions is implemented in the improved NSGA-II. An experiment with ZDT3 is run 30 times repeatedly to test the effect of proposed mechanism. For the repeatability test, the population size and the evolutional generation are set to 100, while the crossover rate equals 0.85 and the mutation rate is set to 0.15. After this computation, no overlapping solutions appear in the solution set of each repetition obtained by the improved algorithm. Among these solution sets, one is exemplified in **Fig. 9** (overlapping points are offset) to be compared with the original NSGA-II.

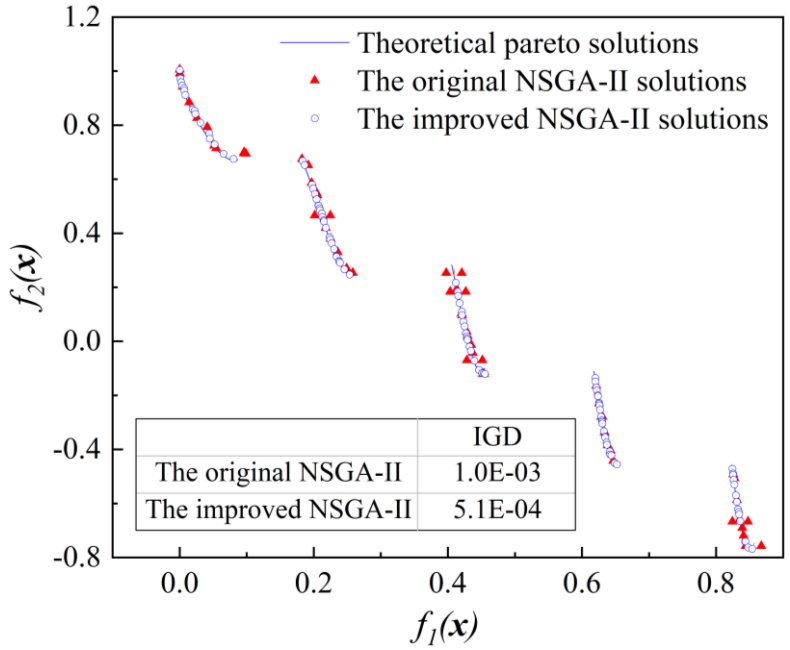

Fig. 9. The effect of the reduction mechanism of overlapping solution on the ZDT3 problem

A performance metric as shown in **Fig. 9**, the inverted generational distance (IGD) (Veldhuizen and Lamont, 2000), is calculated to evaluate the quality of approximations to the true *Pareto* front obtained by the improved NSGA-II. It is defined as:

$$\mathrm{IGD} = \frac{\sum_{\bar{j} \in PF^*} d_{\bar{j}}^{'}}{n} \qquad (4)$$

where $d_{\bar{j}}^{'} = \min_{\bar{i} \in P} \left| \bar{j} - \bar{i} \right|$ is the Euclidean distance between each of the solutions and the closest solution on the true *Pareto* front, and n is the number of non-dominated solutions

obtained. IGD is the measure of the separation between the *Pareto* front and the non-dominated solutions obtained. If all the non-dominated solutions obtained lie on the true *Pareto* front, the value IGD will equal to zero, *i.e.*, the smaller value of IGD indicates the better performance of a MOEA. As presented in **Fig. 9**, the improved NSGA-II has a smaller IGD than the original one, which suggests that it has the better performance.

4.2. **Case 2:** Extractive distillation by varying pressure

The extractive distillation with varying pressure (EDVP) is an energy-efficient separation process of pressure-sensitive azeotropic mixtures. An increasing attention goes to the optimization of these processes since it possesses the advantages of extractive distillation (Hu et al., 2019; Luyben, 2018; Shen et al., 2015; A. Yang et al., 2018; Yang et al., 2019a, 2019c). Recently a particular attention (You et al., 2017) has been focused to the SOO of the EDVP process such as the optimization of operation costs applying the sequence quadratic program (SQP). You *et al*. (2017) presented the analysis of process feasibility and established a certain process (see **Fig. 10**). The system of acetone/methanol with chlorobenzene as entrainer was investigated in the case, where methanol with a higher boiling point was withdrawn as distillate in the extractive column. For the optimization of energy consumption, they proposed an objective function (i.e. the operational cost, f_1, see Eqs.5a) taking both extractive columns and regeneration columns into account simultaneously. After obtaining the optimized result, You *et al*. (2017) also calculated the total annual cost (TAC) in Eq.(5f) to comprehensively evaluate the operating cost and equipment cost. In this section, a different strategy, the multi-objective optimization, was applied to extend solution space for comparing with the results of SOO.

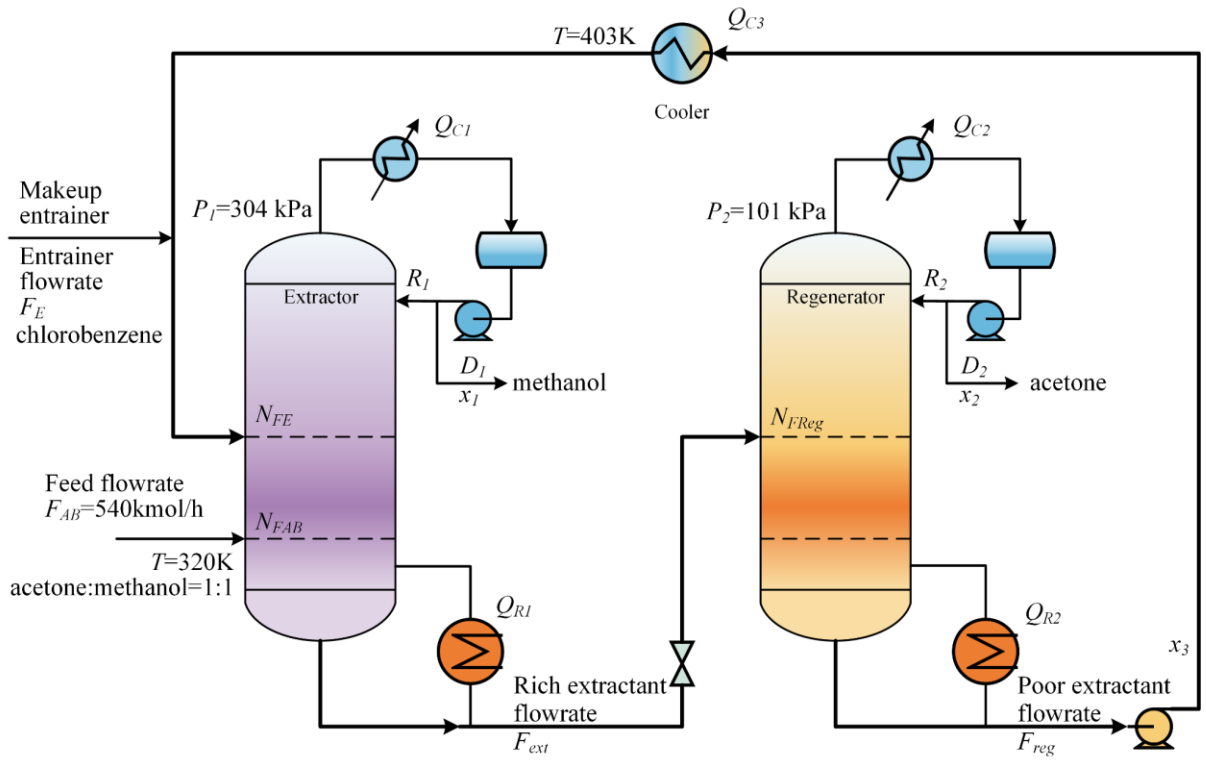

Fig. 10. The flowsheet of the extractive distillation with the notation of variables.

At first, the MOO problem was formulated in this case study. Two conflicting objectives including the operational cost (f_1) and the capital cost (f_2) were optimized. The TAC (Douglas, 1988) was no longer considered as an objective but an important observed variable. The first objective with respect to the total energy cost per unit product is given in Eq. (5a), which involves the heat duties of all re-boilers, coolers of two columns and the entrainer cooler. For calculating the capital cost, the same cost formulas within work conducted by You *et al*. (2017) were employed. The column shell, tray and heat exchanger costs constitute the capital cost, and their formulas are provided in the Eq. (5b) (more details are given in the Supporting Information). In addition, the equimolar feed to be separated (F_{AB} = 540 kmol/ h) and the entrainer feed were set at 320 K for this case, while the same product purity constraints (0.995 molar fractions) of both acetone and methanol were specified. From Eq. (5a) to Eq. (5e) the mathematical formulation of the optimization problem is presented.

Minimize f_1, f_2:

$$f_1 = \frac{M_{R1} \cdot Q_{R1} + m_c \cdot |Q_{C1}| + M_{R2} \cdot Q_{R2} + m_c \cdot |Q_{C2}| + m_c \cdot |Q_{C3}|}{D_1 + k \cdot D_2} \quad (5a)$$

$$f_2 = \frac{\sum_{i=1}^{7} C_{Ei}}{t} \quad (5b)$$

Subject to: (5e)

$$x_{methanol,D_1} \geq 0.995$$

$$x_{methanol,W_1} \leq 0.001$$

$$x_{acetone,D_2} \geq 0.995$$

$$x_{chlorobenzene,W_2} \geq 0.995$$

$$TAC = \frac{\text{capital cost}}{\text{payback period}} + \text{operating cost} = \frac{f_2}{t} + 7200*(M_{R1}Q_{R1} + m_c|Q_{C1}| + M_{R2}Q_{R2} + m_c|Q_{C2}| + m_c|Q_{C3}|) \quad (5f)$$

Before the multi-objective optimization, a SA was implemented for determining the key variables and search space. For the extractive distillation, the larger reflux ratio does not mean the better product quality. Thus, it is necessary to find a reasonable range of reflux ratio with the SA. In this case, as chlorobenzene is a heavy entrainer, the regenerator with a lower pressure can benefit its purification. As such, the condenser pressure of the regenerator was considered as a constant set to 100.0 kPa in the SA. The condenser pressure of the extractive distillation column and the entrainer flowrate were regarded as the manipulated variables while the reflux ratios of two columns, capital cost and operational cost were chosen as the sampled variables. It should be noted that the product purity was constrained in the “Design-spec/Vary” function of Aspen Plus® (the reflux ratios of the two columns were varied) and only the available results are presented in **Fig. 11**. For the effective separation, the reflux ratio needs to be lower while the flowrate of entrainer is kept constant and the condenser pressure is higher (see **Fig. 11a**).

On the other hand, both higher pressures in the condenser of the extractive column and larger entrainer flowrates require the higher reflux ratio in the regeneration column to keep the higher separation efficiency (see **Fig. 11b**), while causing the higher capital and operational costs (see **Fig. 11c and Fig. 11d**). However, it is only feasible to run the extractive column with higher pressures if the entrainer flowrate becomes lower. These results indicate that the optimal solutions may be realized by lower entrainer flowrates or higher condenser pressure of the extractive column.

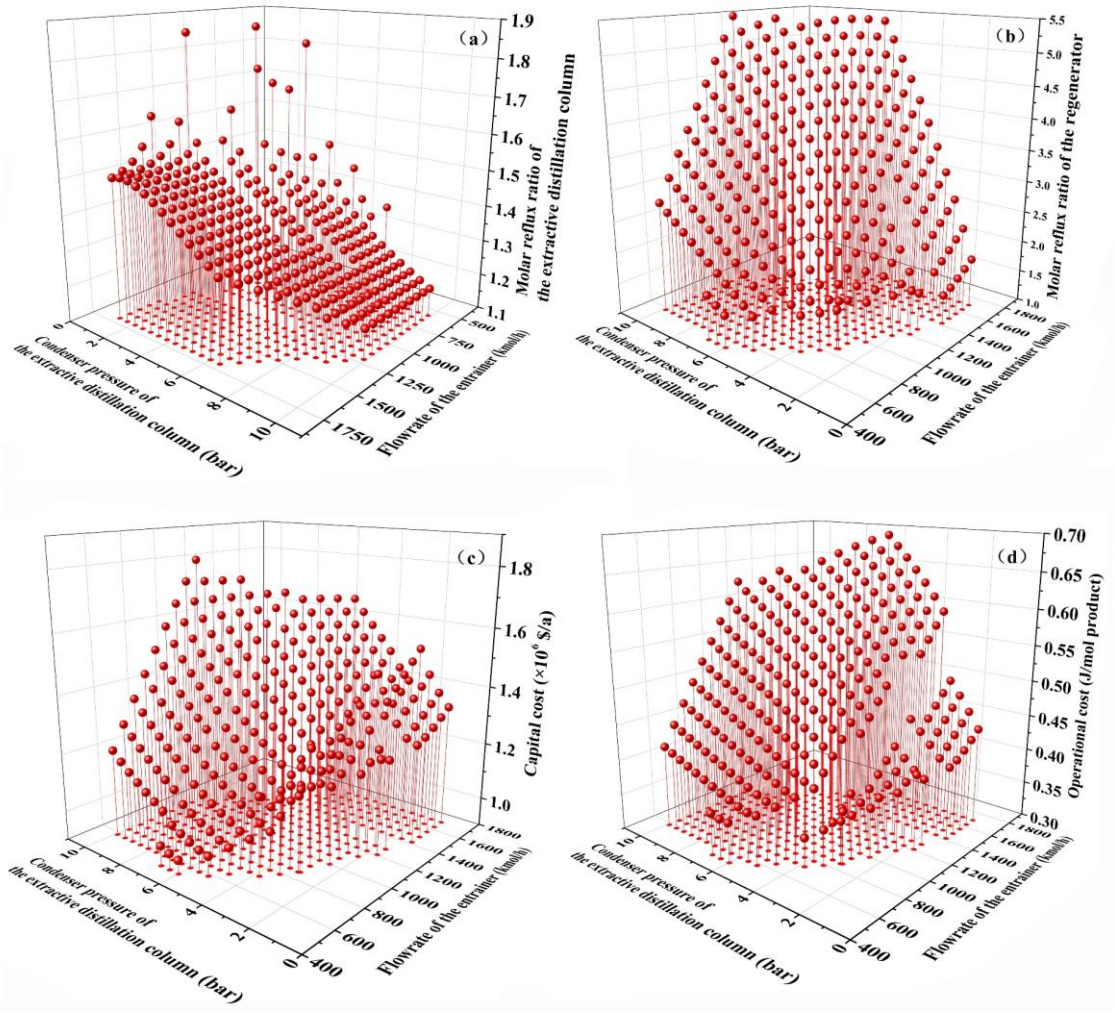

Fig. 11. Effect of the condenser pressure of the extractive distillation and the entrainer flowrate on (a) the required molar reflux ratio of the extractive distillation, (b) the required molar reflux ratio of the regenerator, (c) the capital cost, and (d) the operational cost.

To evaluate the proposed strategy more comprehensively, we formulated three optimization

plans with different ranges of the decision variables including N_{T1}, N_{T2}, F_E, R_1, R_2, D_1, D_2, N_{FE}, N_{FAB}, and N_{FReg}. The first plan was used to explore the optimal solutions of the MOO without a sensitivity analysis (SA) and any preference by the original and improved NSGA-II. After the SA of this process was carried out, the second plan searched the optimal solutions in a more reasonable range of design variables. Finally, the third plan was employed to validate the improved NSGA-II with r-dominance. The decision variables optimized in these plans are shown in **Table 2** while the search space of decision variables is given in **Table 3**.

Table 2 The decision variables optimized in the Case 1.

Decision variables	Symbols
The condenser pressure of the extractive distillation column	P_1
The condenser pressure of the regenerator	P_2
The flowrate of the entrainer	F_E
The reflux ratio of the extractive distillation column	R_1
The reflux ratio of the regenerator	R_2
The distillation flowrate of the extractive distillation column	D_1
The distillation flowrate of the regenerator	D_2
The stage number of the extractive distillation column	N_{T1}
The stage number of the regenerator	N_{T2}
The mixture feed stage of the extractive distillation column	N_{FE}
The entrainer feed stage of the extractive distillation column	N_{FAB}
The feed stage of the regenerator	N_{FReg}

Table 3 The search space of decision variables in Case 1.

Decision variables	1st Plan		2nd Plan with SA		3rd Plan		Units
	Upper limits	Lower limits	Upper limits	Lower limits	Upper limits	Lower limits	
P_1	1000.0	100.0	1000.0	600.0	1000.0	100.0	kPa
P_2	450.0	100.0	250.0	101.0	450.0	100.0	kPa
F_E	1700.0	300.0	600.0	1.0	1700.0	840.0	kmol/h
R_1	3.5	0.95	2.0	0.5	3.5	0.95	-
R_2	5.5	1.35	2.0	0.5	5.5	1.35	-
D_1	272.0	268.0	272.0	268.0	272.0	268.0	kmol/h
D_2	272.0	268.0	272.0	268.0	272.0	268.0	kmol/h

N_{T1}	50	38	50	38	50	38	-
N_{T2}	25	15	25	15	25	15	-
N_{FE}	37	28	37	28	37	28	-
N_{FAB}	25	2	25	2	25	2	-
N_{FReg}	15	25	15	25	15	25	-

For these three plans, the population size was set to 100 individuals and the mutation ratio was considered as 0.2 while the crossover ratio was set as 0.95. A series of solution sets were obtained after 500 iterations were accomplished, all of them for each generation were recorded. **Fig. 12** describes the trend of solution sets for every hundred generations in the first plan. A remarkable decrease of two objectives can be observed from 200 to 500 generations. After 400 generations were iterated, the solution set of 400th generation achieved by the improved NSGA-II were more preferable than that of 500th generation given by the original one. It can be suggested that the improved NSGA-II outperforms the original one. On the other hand, **Fig. 12** also shows the different numbers of overlapping solutions in the solution set generated by the two algorithms while the duplicate copies have been offset for clarity. Obviously, there exist more overlapping solutions in the solution sets achieved by the original NSGA-II, *i.e.*, the improved NSGA-II can achieve a better-distributed solution set.

Further, two solutions presented in **Table 4** are selected as trade-offs respectively from the optimal solution sets achieved by the two algorithms. Comparing these solutions with the result achieved by SOO, there are the less demand of entrainer but the higher operating pressure of extractive distillation. Meanwhile, the operational cost and capital cost (f_1 and f_2) achieved by the improved NSGA-II are also lower than their values in the SOO result. It can be inferred that the higher operating pressure of the extractive distillation and less entrainer could result in the smaller size of equipment and lower energy consumption. Another point should be noted that the search space had reached the boundaries of several variables in the first plan (e.g. the

entrainer flowrate almost equals its lower bound), which implies there may still exist some space to go further in the optimization. As the practical problems may be highly complex, most of the time designers could not be aware of a reasonable decision space at the early stage of MOO. Fortunately, the knowledge provided by SA can help us to reduce the uncertainties of formulating a MOO problem. For example, if the designers have known that the less entrainer and the higher pressure of extractive distillation can bring the lower cost, they may narrow the decision variable space of the first plan. As the second plan shown in **Table 3**, the upper and lower bounds of the entrainer flowrate and operating pressure of the extractive distillation had been adjusted. The results recalculated by the improved NSGA-II with SA include a series of better solutions shown in **Fig. 12**. Although the initial scope of SA is still determined intuitively, the SA can provide an objective trend contributing to understanding the relationships between input and output variables.

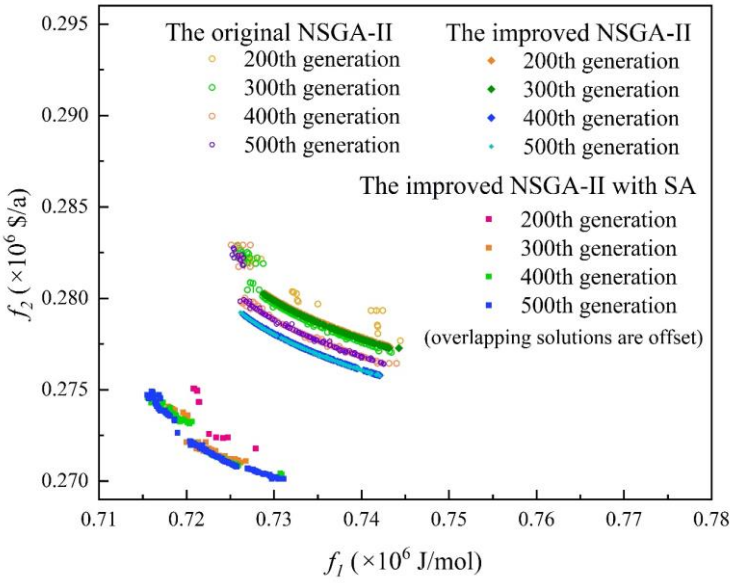

Fig. 12. Evolution trend of solution sets on the MOO problem of all the three plans.

In the third plan, the upper and lower bound of the entrainer flowrate was narrowed into a range closer to the SOO plan, which was to validate the proposed strategy with DM's preference. For comparison, the third plan was optimized without any preference at first. After

400 generations were iterated, the final non-dominated solutions composed of two regions are presented in **Fig. 13a**. When the DM's preference is not introduced, the improved NSGA-II cannot determine the pros and cons of these solutions. If the process designers may be more interested to the solutions in the region 1, and the time consumed by the solutions in the region 2 could be considered as the extra time consumption. Since the TAC is often employed as the objective in the SOO, the TAC values of these solutions are compared between these two regions manually. It can be found that the solutions have the smaller TAC values and the lower capital cost (*i.e.* the smaller equipment size) in the region 1. The reason is that the payback period t can be considered as a parameter to adjust the proportion of capital cost in the TAC shown in Eq. (5f). However, it is tough to weigh the importance of two conflicting objectives in the original NSGA-II. In the proposed strategy, the employment of r-dominance in the improved NSGA-II allows designer to specify a reference point close to region 1 guiding the solution set locating in the preferred region.

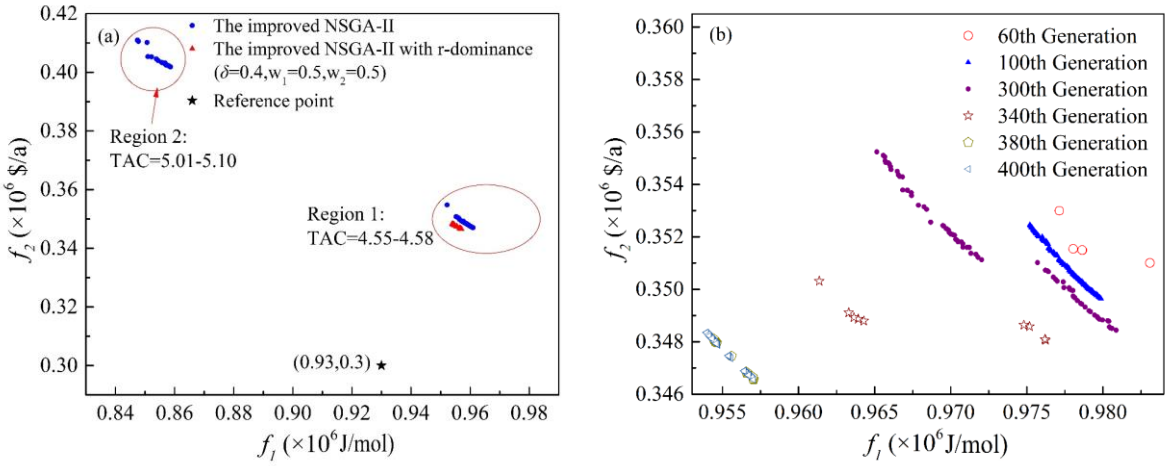

Fig. 13. The distribution of solution sets on the third plan: (a) the optimal solutions of the 400th generation; (b) the evolution trend obtained by r-dominance

The cooperation of the improved NSGA-II with r-dominance needs to specify several additional parameters including a reference point vector $\boldsymbol{r}$, the threshold δ and the weight vector $\boldsymbol{w}$ need to introduce the designer's preference. The extra parameter values in the third plan are

given in **Fig. 13**, and other settings are consistent with the first plan except the entrainer flowrate. After 400 generations were iterated, the improved NSGA-II with r-dominance gave a solution set only appeared in the region 1 rather than in the region 2 (see **Fig. 13b**). Moreover, the solution set obtained with r-dominance are more preferable than the one without any preferences. It can be concluded that the improved NSGA-II with r-dominance can make solutions converge to the region preferred by designers. In other words, the r-dominance could employ the designer's preference in a practical problem of chemical engineering and reach the desired solutions without exploring the whole set of *Pareto* solutions.

Table 4 Comparison among the results achieved by the MOO and SOO of Case 2

Variables and objectives	SOO	1st plan		2nd plan	3rd plan	Units
		Original NSGA-II	Improved NSGA-II	Improved NSGA-II with SA	Improved NSAII with r-dominance	
P_1	300.0	978.7	983.6	974.9	294.1	kPa
P_2	100.0	113.5	116.3	105.0	100.0	kPa
F_E	858.4	300.9	300.0	257.6	840.0	kmol/h
R_1	1.710	1.221	1.209	1.301	1.689	-
R_2	1.702	1.350	1.350	1.165	1.540	-
D_1	271.0	270.8	270.8	270.8	270.5	kmol/h
D_2	270.8	271.0	271.0	271.1	268.1	kmol/h
N_{T1}	45	47	48	48	45	-
N_{T2}	18	17	17	17	15	-
N_{FAB}	36	36	36	37	36	-
N_{FE}	18	19	20	18	17	-
N_{FReg}	6	7	7	7	6	-
$x_{m,D1}$	0.995	0.995	0.995	0.995	0.995	-
$x_{m,W1}$	3.0e-4	0.001	0.001	0.001	0.001	-
$x_{a,D2}$	0.996	0.995	0.995	0.995	0.995	-
$x_{c,W2}$	1.000	1.000	1.000	1.000	1.000	-
f_1	0.356	0.278	0.277	0.272	0.347	J/mol
f_2	1.020	0.734	0.732	0.723	0.957	10^6 \$/a
TAC	4.720	3.603	3.597	3.528	4.520	10^6 \$/a

This case study presents the advantages of the improved algorithm from two aspects. One is to improve the search efficiency of NSGA-II by suppressing the generation of redundant solutions, and the other is to control the evolution direction by introducing the DM's preferences. Finally, the increase in efficiency will be reflected in the reduction of time consumption. As shown earlier, the improved algorithm outperformed, in which either the same number of generations led to a more preferable solution set, or a better solution set needed fewer iterations. For all these plans, it took an average of 1.7 minutes to compute each generation for the improved and original NSGA-II while the time was saved by reducing the number of iterations. And also, the SA is helpful to find a suitable decision space at the early stage of MOO, it can further make optimization more purposeful.

4.3. **Case 3:** Methanol synthesis loop

The effectiveness of the improved NSGA-II with r-dominance had been verified in the previous bi-objective case. However, there may exist the problems with more than two objectives, *e.g.*, the global optimization considering the factors of economics, environment, productivity. As methanol is one of the most promising renewable energy to replace the fossil fuels, the methanol production has been a research hotspot (Y. Yang et al., 2018). A process of methanol synthesis shown in **Fig. 14** is exemplified to be optimized with the improved algorithm. The case study is a more complex problem involving three objectives for comparing the two different preference-based NSGA-II (*i.e.* r-dominance and A-dominance). The mathematical model was formulated including three objectives: the operational cost (J_1), the capital cost (J_2) and the opposite of total carbon efficiency (J_3). The critical indicator of the production efficiency, total carbon efficiency, can be calculated as the ratio between the mass of carbon atoms in the product and the mass of carbon atoms in the fresh feed. In this process,

the methanol reactor was simulated with a reaction kinetic model (Vanden Bussche and Froment, 1996). Moreover, the quality of the product methanol was not considered as an objective but a constraint. The main units including a methanol reactor, a compressor, one flash vessel, heat exchangers, and a washing column are counted in the capital cost. From Eq. (6a) to Eq. (6d), the mathematical formulation of the optimization problem is presented (more details are given in the Supporting Information), and the feed composition of the fresh syngas is listed in the **Table 5**. Besides, the TAC (Eq. (6e)) was still considered as an indicator of reference but not as an objective.

$$J_1 = (M_2 ? P_{COMP} + m_c' \bullet |Q_C|) \times 7200 \quad (6a)$$

$$J_2 = \sum_{i=1}^{7} C_{mi} \quad (6b)$$

$$J_3 = 1 - \frac{F_{CH_4O}}{F_{CO} + F_{CO_2}} \quad (6c)$$

Note: $P_{COMP} > 0$, $Q_C < 0$

Minimize $J_1 \quad J_2 \quad J_3$

subject to: $1.0 \geq x_{CH_4O,product} \geq 0.6$ (6d)

$$TAC = \frac{\text{capital cost}}{\text{payback period}} + \text{operating cost} = \frac{J_2}{t} + J_1 \quad (6e)$$

Table 5 Feed composition of the fresh syngas in Case 3.

Components	Molar fraction (%)
CO_2	3.500
CH_4	0.690
H_2	69.560
CO	23.290
N_2	2.960

As methanol synthesis reactions are reversible and exothermic, the coolant temperature (T_1) and the feed temperature (T_2) of the methanol reactor were chosen as two decision variables.

Meanwhile, the flowrate (F_R) of the recycle syngas has a noticeable impact to the power consumption of the compressor, which was also used as a significant variable in the problem. The hydrogen recovery system was simplified to a SEP unit in Aspen Plus® and its recovery ratio (E_1) was considered as a decision variable as well. Washing water can reduce the methanol in the recycle syngas and purge gas but it works to the disadvantage of the purity of crude methanol and the operational cost. On the other hand, equipment dimensions are crucial to the total capital cost and the performance of a whole process. Among the devices, the methanol reactor cannot be sized automatically in the process simulator while the other devices including heat exchangers and columns can be sized by the process simulator. Thus, the size of the reactor was also considered as an optimized variable. For clarity, all decision variables are summarized in **Table 6**.

Table 6 The decision variables optimized in the methanol synthesis loop

Optimized parameters		Upper limits	Lower limits	Units
Temperature of the coolant in methanol convertor	T_1	255	203	℃
Temperature of preheater outlet at the cold-side	T_2	220	190	℃
Flowrate of the recycle syngas	F_R	9500	1800	kmol/h
Flowrate of the washing water	F_w	6500	500	kg/h
hydrogen recovery ratio	E_1	0.950	0.010	-
Number of the tube in methanol converter	N_1	4500	1500	-

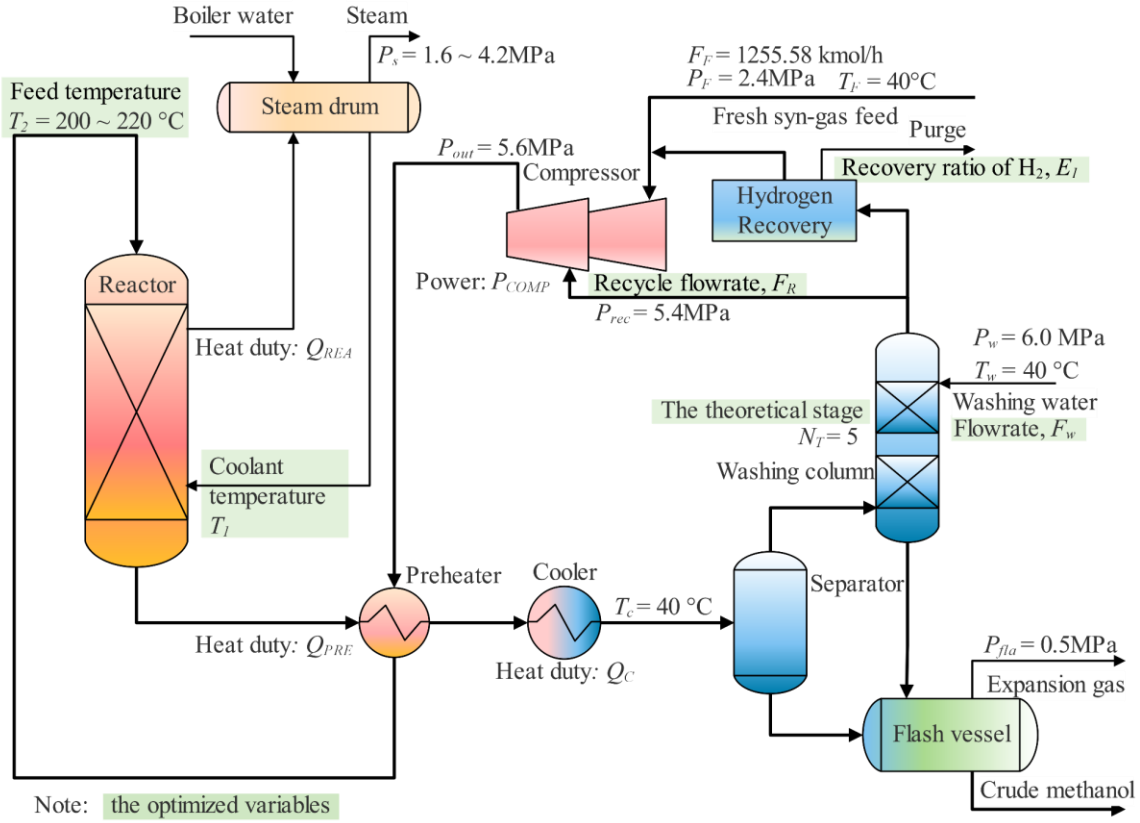

Fig. 14. The flowsheet of the methanol synthesis loop with the notation of variables.

The improved NSGA-II was used to solve this case with three configurations: without any preference, with r-dominance and with A-dominance. For the parameters of each configuration, the population included 100 individuals and the mutation probability was considered as 0.2 while the crossover ratio was set as 0.95. After 100 generations were iterated, the optimal solutions depicted in **Fig. 15** were obtained. As a designer often selects a solution as the trade-off from the region in the green circle of **Fig. 15a**, the solutions outside the green circle may consume the extra time. To introduce the DM's preference, the improved algorithms with r-dominance and A-dominance are used to optimize the process respectively. Unfortunately, the solutions cannot be converged in the designer's preferred region by the NSGA-II with r-dominance (see **Fig. 15b**) while they almost stay in the objective space without any preferences. In contrast, the solutions achieved by the NSGA-II with A-dominance are converged in the

preferred region (see **Fig. 15c and Fig. 15d**).

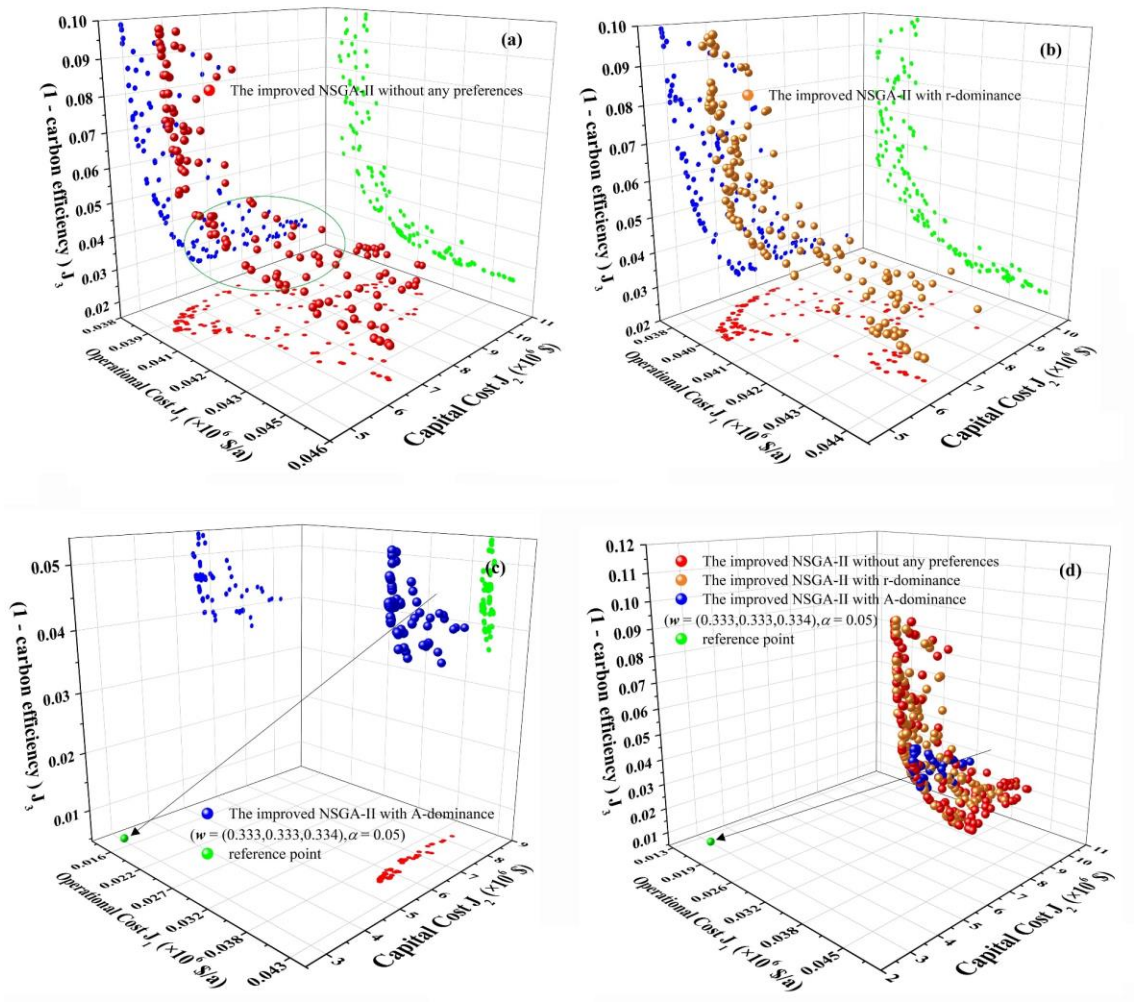

Fig. 15. The optimal solutions of this tri-objective case: (a) the improved NSGA-II without any preferences (b) the improved NSGA-II with r-dominance (c) the improved NSGA-II with A-dominance and (d) the comparison of above all

In this case study, the solution sets have a strong concave behavior on the *Pareto* front, thus it is convenient to choose a trade-off solution for the designers. In other words, there exists a region including some trade-off solutions that can increase the carbon efficiency and keep a relatively low operational and capital cost. As such, one solution near the most concave of this region was picked out as the final solution and presented in **Table 7**. When the DMs have an interest in this region, they could control the convergence of solutions with the assist of A-dominance. However, the extra parameters including the position of reference points and the

threshold should be determined carefully, since they have significant impacts on the search space of optimization.

Table 7 The final determined solutions of Case 3 from the optimal set.

Design parameters, product quality and cost data			Units
Temperature of the coolant in methanol convertor	T_1	240.5	℃
Temperature of preheater outlet at the cold-side	T_2	200.1	℃
Flowrate of the recycle syngas	F_R	3138	kmol/h
Flowrate of the washing water	F_w	662.7	kg/h
hydrogen recovery ratio	E_1	7.676e-4	-
Number of the tube in methanol converter	N_1	1779	-
Operational cost	J_1	0.03972	10^6 \$/a
Capital cost	J_2	5.197	10^6 \$
the carbon efficiency	1.0-J_3	0.9332	-
Total annual cost	TAC	1.772	10^6 \$/a
Methanol production	F_M	10058	kg/h
Molar fraction of the methanol in the product	x_M	0.8844	-

After all computations were finished, it took a long time to invoke the developed algorithms with the process simulator. Statistically, each generation needed approximately 11 minutes to calculate in these three configurations, *i.e.*, the computation of 100 generations took approximately 18 hours. In fact, the solutions obtained by A-dominance had begun to fall into the preferred region while r-dominance cannot guide the solutions efficiently even running 100-generation iteration. As such, the improved NSGA-II with A-dominance could be potentially more effective preference-based algorithm than that with r-dominance for the cases with high-dimensional objectives. Nevertheless, most computing time was consumed in achieving convergence of the process model, especially for the process with plenty of iterative loops. It indicates that the model complexity in a process simulator has significant influence on the computational performance.

5. Conclusion

In this work, a strategy was proposed to search the desirable solutions for the MOO problems of chemical processes, which allows designers to control the distribution of solutions according to their knowledge and experience. In the proposed strategy, the improved NSGA-II as the key technique, has two significant advantages: the improved non-dominated sorting with a designer's preference, and the mechanism for reducing overlapping solutions. To introduce designer's preference, two dominant relationships involving r-dominance and A-dominance were integrated into NSGA-II. For the improved NSGA-II with r-dominance, a reference point was used to control the direction of convergence and the weights are employed to control the bias of solutions. By contrast, the NSGA-II with A-dominance employs an angle to represent a designer's preference. From a mathematical perspective, both of the two algorithms work effectively to three test functions in the first case study while the improved NSGA-II can also obtain fewer overlapping solutions than the original one.

For the practical issues of chemical processes, the improved NSGA-II was validated and highlighted by two illustrative cases. A case of extractive distillation was exemplified for the proposed strategy, in which the better convergence of the improved NSGA-II was presented. The results also suggest the necessity of SA carried out for reducing the blindness at the model formulation. Moreover, the designer's preference was introduced to obtain the smaller TAC by r-dominance with effect. And the other one case is a more complex problem, a methanol synthesis loop with three objectives. Both r-dominance and A-dominance were applied to the tri-objective case with the improved NSGA-II. The result reveals that the r-dominance cannot make the solutions converge into the desirable region but the A-dominance can achieve the desired effect. It is also suggested that the A-dominance is more suitable for the tri-objective problems, and r-dominance could be employed to optimize bi-objective problems.

Although we have to admit that the final solution for a problem still relies on the final decision of designers, the proposed strategy could help them to find their desirable solution effectively. The overall purpose of this work is to draw the attention of the process designers to the preference-based MOEAs with SA, particularly from the community of process systems engineering, to reduce time-consumption using the methods discussed in this work. In the future work, the strategy optimizing the MOO problems with the discrete variables still need to be studied and the method to determine the parameters representing the designer's preference should be also explored further.

Acknowledgement

We acknowledge the financial support provided by the National Natural Science Foundation of China (Nos. 21878028, 21606026); the Fundamental Research Funds for the Central Universities (No. 2019CDQYHG021); the Beijing Hundreds of Leading Talents Training Project of Science and Technology (No. Z171100001117154).

Nomenclature

$f(\boldsymbol{x}), f_i, J_i$	objective functions, fitness functions
$f_i^{\max}$, $f_i^{\min}$	the maximum, minimum fitness function in the current population
$\boldsymbol{x}^L$	the vectors representing the lower constraints
$\boldsymbol{x}^U$	the vectors representing the upper constraints
$h(\boldsymbol{x})$	the equality in a MOO formulation
$g(\boldsymbol{x})$	the inequality in a MOO formulation
$\boldsymbol{P}$	a population of individuals
$\boldsymbol{g}$	the vector representing a reference point

$\boldsymbol{w}$ a weight vector of objectives

A an individual (point A) in the population

B an individual (point B) in the population

X an individual (point X) in the population

Y an individual (point Y) in the population

$D(A, B, \boldsymbol{g})$ the relative difference between the distance from A to $\boldsymbol{g}$ and the distance from B to $\boldsymbol{g}$

$Dist_{\max}$ the maximum distance from $\boldsymbol{g}$ to the farthest point in the population

$Dist_{\min}$ the minimum distance from $\boldsymbol{g}$ to the closest point in the population

$Dist(A, \boldsymbol{g})$ the Euclidean distance between A and $\boldsymbol{g}$

δ the non-r-dominance threshold

$\boldsymbol{b}$ a vector representing the ideal point

$\boldsymbol{i}$ the relative distance between X and $\boldsymbol{b}$

$\boldsymbol{j}$ the relative distance between Y and $\boldsymbol{b}$

$Angle(X, Y)$ the angle between X and Y

$Angle(X, \boldsymbol{g})$ the angle between X and $\boldsymbol{g}$

$Angle(Y, \boldsymbol{g})$ the angle between X and $\boldsymbol{g}$

PF^* the true *Pareto* front

$d'_{\bar{j}}$ the Euclidean distance between each solution and the closest solution on the PF^*

$\bar{j}$ each solution

$\bar{i}$ the closet solution to the solution $\bar{j}$

k	the price difference ratio of two distillates
M_{R1}, M_{R2}	the energy price ratio of the steam used in the reboilers
m_c	the energy price ratio of the cooling water used in the coolers of Case 2
m_c'	the energy price of the cooling water used in the coolers of Case 3
C_{Ei}	the capital cost of each device in the case 1, $
t	payback period, year
Q_R	the heat duties of the reboilers, GJ/h
Q_C	the heat duties of the condensors, GJ/h
C_{mi}	the capital cost of each device in the case 3, $
F_{CH4O}	the molar flowrate of product methanol, kmol/h
F_{CO}	the molar flowrate of carbon monoxide in the fresh gas, kmol/h
F_{CO2}	the molar flowrate of carbon dioxide in the fresh gas, kmol/h
P_{COMP}	the power of the compressor in the case 3, GJ/h

References

Beykal, B., Boukouvala, F., Floudas, C.A., Pistikopoulos, E.N., 2018. Optimal design of energy systems using constrained grey-box multi-objective optimization. Comput. Chem. Eng. 116, 488–502. https://doi.org/10.1016/J.COMPCHEMENG.2018.02.017

Biegler, L.T., Grossmann, I.E., 2004. Retrospective on optimization. Comput. Chem. Eng. 28, 1169–1192. https://doi.org/10.1016/J.COMPCHEMENG.2003.11.003

Binh, T.T., Korn, U., 1997. MOBES: A multiobjective evolution strategy for constrained optimization problems. Proc. Third Int. Conf. Genet. Algorithms (Mendel ’97) 25, 176–182. https://doi.org/10.1.1.46.8661

Bortz, M., Burger, J., Asprion, N., Blagov, S., Böttcher, R., Nowak, U., Scheithauer, A., Welke, R., Küfer, K.H., Hasse, H., 2014. Multi-criteria optimization in chemical process design and decision support by navigation on Pareto sets. Comput. Chem. Eng. 60, 354–363. https://doi.org/10.1016/j.compchemeng.2013.09.015

Branke, J., Kauûler, T., Schmeck, H., 2001. Guidance in evolutionary multi-objective optimization. Adv. Eng. Softw. 32, 499–507. https://doi.org/10.1016/s0965-9978(00)00110-1

Chankong, V., Y. Haimes, Y., 1983. Multiobjective decision making: theory and methodology. North-Holland, New York, p. 406.

Coello, C.A.C., 2000. Handling preferences in evolutionary multiobjective optimization: a survey, in: Dahal KP, Burt G, Mcdonald J, G.S. (Ed.), Proceedings of the 2000 congress on evolutionary computation. CEC00 (Cat. No.00TH8512). IEEE, pp. 30–37. https://doi.org/10.1109/CEC.2000.870272

Coello, C.A.C., Lamont, G.B., Veldhuizen, D.A. Van, 2007. Evolutionary algorithms for solving multi-objective problems, 2nd ed. Springer, Boston. https://doi.org/10.1007/978-0-387-36797-2

Datta, S., Dev, V.A., Eden, M.R., 2017. Hybrid genetic algorithm-decision tree approach for rate constant prediction using structures of reactants and solvent for Diels-Alder reaction. Comput. Chem. Eng. 106, 690–698. https://doi.org/10.1016/J.COMPCHEMENG.2017.02.022

Deb, K., 2011. Multi-objective optimisation using evolutionary algorithms: An introduction, in: Wang Lihui, Ng Amos H. C., D.K. (Ed.), Multi-objective evolutionary optimisation

for product design and manufacturing. Springer London, London, pp. 3–34. https://doi.org/10.1007/978-0-85729-652-8_1

Deb, K., Pratap, A., Agarwal, S., Meyarivan, T., 2002. A fast and elitist multiobjective genetic algorithm: NSGA-II. IEEE Trans. Evol. Comput. 6, 182–197. https://doi.org/10.1109/4235.996017

Garcia, D.J., You, F., 2015. Multiobjective optimization of product and process networks: General modeling framework, efficient global optimization algorithm, and case studies on bioconversion. AIChE J. 61, 530–554. https://doi.org/10.1002/aic.14666

Greco, S., Ehrgott, M., Figueira, J., 2005. Multiple criteria decision analysis : state of the art surveys. Springer, New York, NY. https://doi.org/10.1007/b100605

Habibi, H., Chitsaz, A., Javaherdeh, K., Zoghi, M., Ayazpour, M., 2018. Thermo-economic analysis and optimization of a solar-driven ammonia-water regenerative Rankine cycle and LNG cold energy. Energy 149, 147–160. https://doi.org/10.1016/J.ENERGY.2018.01.157

He, C., You, F., 2015. Process design and optimization of an integrated shale gas process for green chemicals production. Comput. Aided Chem. Eng. 37, 1397–1402. https://doi.org/10.1016/B978-0-444-63577-8.50078-4

Herring Iii, R.H., Eden, M.R., 2015. Evolutionary algorithm for de novo molecular design with multi-dimensional constraints. Comput. Chem. Eng. 83, 267–277. https://doi.org/10.1016/j.compchemeng.2015.06.012

Hu, Y., Su, Y., Jin, S., Chien, I., Shen, W., 2019. Systematic approach for screening organic and ionic liquid solvents in homogeneous extractive distillation exemplified by the tert-

butanol dehydration. Sep. Purif. Technol. 211, 723–737. https://doi.org/10.1016/j.seppur.2018.10.030

Ishibuchi, H., Narukawa, K., Nojima, Y., 2005. Handling of overlapping objective vectors in evolutionary multiobjective optimization. Int. J. Comput. Intell. Res. 1, 1–18. https://doi.org/10.5019/j.ijcir.2005.19

Khurana, M., Farooq, S., 2019. Integrated adsorbent process optimization for minimum cost of electricity including carbon capture by a VSA process. AIChE J. 65, 184–195. https://doi.org/10.1002/aic.16362

Luyben, W.L., 2018. Control of heat-integrated extractive distillation processes. Comput. Chem. Eng. 111, 267–277. https://doi.org/10.1016/j.compchemeng.2017.12.008

Muñoz López, C.A., Telen, D., Nimmegeers, P., Cabianca, L., Logist, F., Van Impe, J., 2018. A process simulator interface for multiobjective optimization of chemical processes. Comput. Chem. Eng. 109, 119–137. https://doi.org/10.1016/j.compchemeng.2017.09.014

Parhi, S.S., Rangaiah, G.P., Jana, A.K., 2019. Vapor recompressed batch distillation: Optimizing reflux ratio at variable mode. Comput. Chem. Eng. 124, 184–196. https://doi.org/10.1016/J.COMPCHEMENG.2019.02.014

Rangaiah, G.P., 2009. Multi-objective optimization: techniques and applications in chemical engineering (Advances in process systems engineering vol.1), World Scientific, Danvers. https://doi.org/10.1142/7088

Said, L. Ben, Bechikh, S., 2010. The r-dominance: a new dominance relation for interactive evolutionary multicriteria. IEEE Trans. Evol. Comput. 14, 801–818.

https://doi.org/10.1109/tevc.2010.2041060

Segovia-Hernández, J.G., Gómez-Castro, F.I., 2017. Stochastic process optimization using Aspen Plus®. CRC Press, Boca Raton.

Shen, W., Dong, L., Wei, S., Li, J., Benyounes, H., You, X., Gerbaud, V., 2015. Systematic design of an extractive distillation for maximum-boiling azeotropes with heavy entrainers. AIChE J. 61, 3898–3910. https://doi.org/10.1002/aic.14908

Srinivas, N., Deb, K., 1994. Muiltiobjective optimization using nondominated sorting in genetic algorithms. Evol. Comput. 2, 221–248. https://doi.org/10.1162/evco.1994.2.3.221

Vallerio, M., Vercammen, D., Van Impe, J., Logist, F., 2015. Interactive NBI and (E)NNC methods for the progressive exploration of the criteria space in multi-objective optimization and optimal control. Comput. Chem. Eng. 82, 186–201. https://doi.org/10.1016/j.compchemeng.2015.07.004

Vanden Bussche, K.M., Froment, G.F., 1996. A steady-state kinetic model for methanol synthesis and the water gas shift reaction on a commercial $Cu/ZnO/Al_2O_3$ catalyst. J. Catal. 161, 1–10. https://doi.org/10.1006/jcat.1996.0156

Veldhuizen, D.A. Van, Lamont, G.B., 2000. Multiobjective evolutionary algorithms : Analyzing the state-of-the-art. Evol. Comput. 8, 125–147. https://doi.org/10.1162/106365600568158

Wang, P., Emmerich, M., Li, R., Tang, K., Bäck, T., Yao, X., 2015. Convex hull-based multiobjective genetic programming for maximizing receiver operating characteristic performance. IEEE Trans. Evol. Comput. 19, 188–200.

https://doi.org/10.1109/tevc.2014.2305671

Wang, S., Ali, S., Yue, T., Liaaen, M., 2018. Integrating weight assignment strategies with NSGA-II for supporting user preference multiobjective optimization. IEEE Trans. Evol. Comput. 22, 378–393. https://doi.org/10.1109/TEVC.2017.2778560

Xie, Z., Zheng, J., Zou, J., 2012. A-Dominance: angle based preference multi-objective evolutionary algorithm. Int. J. Adv. Comput. Technol. 4, 265–273. https://doi.org/10.4156/ijact.vol4.issue10.31

Yan, N., Ren, B., Wu, B., Bao, D., Zhang, X., Wang, J., 2016. Multi-objective optimization of biomass to biomethane system. Green Energy Environ. 1, 156–165. https://doi.org/10.1016/J.GEE.2016.05.001

Yang, A., Shen, W., Wei, S., Dong, L., Li, J., Gerbaud, V., 2019a. Design and control of pressure-swing distillation for separating ternary systems with three binary minimum azeotropes. AIChE J. 65, 1281–1293. https://doi.org/10.1002/aic.16526

Yang, A., Sun, S., Eslamimanesh, A., Wei, S., Shen, W., 2019b. Energy-saving investigation for diethyl carbonate synthesis through the reactive dividing wall column combining the vapor recompression heat pump or different pressure thermally coupled technique. Energy 172, 320–332. https://doi.org/10.1016/j.energy.2019.01.126

Yang, A., Wei, R., Sun, S., Wei, S., Shen, W., Chien, I.L., 2018. Energy-saving optimal design and effective control of heat integration-extractive dividing wall column for separating heterogeneous mixture methanol/toluene/water with multiazeotropes. Ind. Eng. Chem. Res. 57, 8036–8056. https://doi.org/10.1021/acs.iecr.8b00668

Yang, A., Zou, H., Chien, I.L., Wang, D., Wei, S., Ren, J., Shen, W., 2019c. Optimal design

and effective control of triple-column extractive distillation for separating ethyl acetate/ethanol/water with multiazeotrope. Ind. Eng. Chem. Res. 58, 7265–7283. https://doi.org/10.1021/acs.iecr.9b00466

Yang, Y., Liu, J., Shen, W., Li, J., Chien, I.L., 2018. High-efficiency utilization of CO_2 in the methanol production by a novel parallel-series system combining steam and dry methane reforming. Energy 158, 820–829. https://doi.org/10.1016/j.energy.2018.06.061

You, X., Gu, J., Peng, C., Shen, W., Liu, H., 2017. Improved design and optimization for separating azeotropes with heavy component as distillate through energy-saving extractive distillation by varying pressure. Ind. Eng. Chem. Res. 56, 9156–9166. https://doi.org/10.1021/acs.iecr.7b00687

Zhu, Y., Xie, J., Zheng, J., Luo, B., Li, W., 2009. Research on overlapping individuals in MOEAs: Causation, probability for quantity and influence on assessment. 6th Int. Conf. Fuzzy Syst. Knowl. Discov. FSKD 2009 2, 14–19. https://doi.org/10.1109/FSKD.2009.24