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A modified DIRECT algorithm for hidden constraints in an LNG process optimization

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ABSTRACT

Optimization for process design in the chemical engineering industry has been important for energy efficiency and economic feasibility. Because many industries perform optimization with a commercial process simulator such as the Aspen HYSYS, an optimization methodology for expensive black-box functions is needed. Thus, the development of derivative free optimization algorithms has long been studied and the deterministic global search algorithm DIRECT (DIviding a hyper-RECTangle) was suggested. In this paper, a modified DIRECT algorithm with a sub-dividing step for considering hidden constraints is proposed. The effectiveness of the algorithm is exemplified by its application to a cryogenic mixed refrigerant process using a single mixed refrigerant for natural gas liquefaction and its comparison with a well-known stochastic algorithm (GA, PSO, SA), and model based search algorithm (SNOBFIT), local solver (GPS, GSS, MADS, active-set, interior-point, SQP), and other hidden constraint handling methods, including the barrier approach and the neighborhood assignment strategy. Optimal solution calculated by the proposed algorithms decreases the specific power required for natural gas liquefaction to 18.9% compared to the base case.

1. Introduction

The chemical process systems are troublesome problems to optimize them because of its essential attributes. They have number of equality constraints such as mass balance and energy balance and it make hard to find a feasible solution. Not only the object function but also the feasible region are generally non-linear, and numerous local optimums exist. To solve these problems, various kinds of optimization algorithms have been developed and applied to the industrial applications [1–8]. Derivative-free optimization, which can optimize the function for which derivative information is unavailable, unreliable, or impractical to obtain because of being expensive to calculate or noisy [9], is the key technique for this purpose. The reason why this kind of technique is important is that many analyzing methodologies used in engineering and science problems are black-box models for which a user cannot get the equations and other specific information being used from either the software or the analyzing machine. Especially, commercial software usually does not give exact equations and derivative information because of calculation methodology or their intellectual property rights. To solve this problem, many researchers have studied derivative-free optimization to optimize their specific engineering or science problems [10–14]. Derivative-free optimization algorithms can be classified by two types of criteria, which are optimizing directly or indirectly and locally or globally. The direct search method uses the objective function directly for optimization whereas models based on an indirect search method regress the original function into an accurate surrogate model. Specifically, nature-inspired metaheuristic stochastic global search algorithms such as a genetic algorithm (GA[1]), simulated annealing (SA), and particle swarm algorithms (PSO) are different from deterministic algorithm because they involve randomness which does not exist in deterministic algorithm. Furthermore, algorithms are different depending on whether their target is local or global. A brief

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[1] All abbreviations are defined in Nomenclature section of this document.

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Table 1
Classification of derivative-free optimization.

		Local Search	Global Search
Deterministic algorithm	Direct search method	Nelder-Mead simplex algorithm	Lipschitzian-based partitioning techniques
		Generalized pattern search (GPS)	- DIvide a hyper-RECTangle (DIRECT)
		Generating set search (GSS)	- Branch-and-Bound (BB] search
		Mesh adaptive direct search (MADS)	Multilevel coordinate search (MCS)
		Pattern search methods using simplex gradient	
	Model-based search method	Trust-region methods	Response surface methods (RSMs)
		Implicit filtering	- Kriging
			- Analysis of computer experiments (DACE) stochastic model
			- Efficient global optimization (EGO)
			- Radial basis functions
			- Sequential design for optimization (SDO)
			Surrogate management framework (SMF)
			Optimization by branch-and-fit
Stochastic algorithm			Hit-and-run algorithms
			Simulated annealing (SA)
			Genetic algorithms (GA)
			Particle swarm algorithms (PSO)

classification of derivative-free optimization algorithms originally provided from Ref. [9] is listed in Table 1 and see Ref. [9] for more details.

In the case of chemical engineering industry, commercial process simulators for designing process systems such as Aspen Plus, Aspen HYSYS, and SimSci PRO/II can be classified as black-box models in general. Since they are sequential modular-based simulators, it is hard to get derivative information of the target variables. Furthermore, an optimization tool given by a program usually shows low performance. Hence, for optimizing the process simulator function, an appropriate derivative-free optimization algorithm is necessary. For this reason, much research has been conducted for designing optimal process models with high-performance, derivative-free optimization algorithms by integrating commercial simulators and optimization algorithms. Lee et al. [15] integrated Aspen Plus and a gradient-based optimization method with MATLAB code for maximizing the exergy efficiency of the multi-component organic Rankine cycle (ORC) by changing component composition. Also, Lee et al. [16,17] used GA for decomposing the MINLP problem to optimize a superstructure of a rigorous rate-based reactive distillation model and green-field post-combustion CO_2 capture process. For optimizing a rigorous tray-by-tray distillation column model, Javaloyes-Antón et al. [18] implanted a particle swarm algorithm into a process model simulated by Aspen HYSYS. Cozad et al. [19] developed the automated learning of algebraic models for optimization (ALAMO) to make a surrogate model of the given derivative-free function, and it can be used for a simulation of model-based derivative-free optimization [20]. Shi and You [21] proposed a novel adaptive surrogate modeling-based algorithm to solve the integrated scheduling and dynamic optimization problem for sequential batch processes. Quirante et al. [22] used kriging interpolation, one of the response surface methods (RSMs), for rigorous designing of distillation columns where original model is formulated by Aspen HYSYS. Not only that, but also various researchers have tried to optimize the process systems using commercial simulator with external optimization algorithms [23–29].

Especially, liquefied natural gas (LNG), which is a widely used energy source for the remote transportation due to its environmental friendly attributes [30,31], is the key area for this type of optimization. The liquefaction process for natural gas (NG) is an energy intensive process and therefore many researchers have widely studied about the process design and optimization of a liquefaction process [32–34]. Among the liquefaction technologies, single mixed refrigerant (SMR) liquefaction process is a traditional but still effective process for many projects with small-scale LNG production capacity [35–37]. It uses only single cycle of mixed refrigerant (MR) and therefore its efficiency is limited compared to the advanced processes such as the propane precooled mixed refrigerant (C3MR) or dual mixed refrigerant liquefaction process. However, it has the advantage of simple configuration, which makes the process easy to operate it with lower capital investment. Also, the efficiency of SMR can be improved with proper modification and optimization, and therefore many researchers have studied about the SMR process optimization problems. Shirazi and Mowla modeled optimized the PRICO SMR process by using GA [38]. Xu et al. modeled and optimized the PRICO SMR with Aspen Plus and GA [39]. Khan et al. modeled a SMR liquefaction process with a commercial simulator Honeywell UniSim Design and optimized it with the nonlinear programming [40], particle swarm paradigm [41] and sequential coordinate random search (modeled by Aspen HYSYS) [42]. Moein et al. modeled the APCI SMR process with Aspen HYSYS and optimized it with GA when the ambient temperature is changed [43]. Morosuk et al. modeled PRICO SMR with Aspen Plus and discussed about the evaluation and optimization for improvement [44]. Mehrpooya and Ansarinasab modeled and compared Linde and APCI liquefaction process based on exergy and cost analysis with Aspen HYSYS [45]. Park et al. modeled and optimized SMR using Aspen HYSYS and particle swarm algorithm with varying ambient temperature [46].

Previous optimization methods for a process simulator usually used a stochastic solver and surrogate model-based optimization because their implementation is simple compared to deterministic algorithms. Especially, nature-inspired metaheuristic algorithms were applied to general purpose of a significant number of process systems studies and they gave fine best found solution in general [16,39,47–54]. However, when optimizing a process with a methodology that has been traditionally used, the following problems may arise. In the case of stochastic solvers, the algorithms highly depend on tuning parameters and the convergence rate of the objective function is slower with improper parameters. In addition, because these parameters are so numerous, finding an appropriate parameter set can be another problem. If the objective function has a high computation cost, it can be very inefficient because

additional evaluation must be applied. Moreover, because of the features of the stochastic solver, randomness, even if the same initial conditions such as population for GA and swarm for PSO are set the same, it can be optimized along with other trajectories, thus causing reproducibility problems. There is also a problem because the initial population itself can have a large impact on optimization and does not guarantee that solvers converge into a global optimal solution. Moreover, although model-based search methods have been developed by machine learning technology, it is difficult to consider hidden constraints, especially complicated shape constraints that should be calculated in a process simulator. In fact, in order to solve these problems, stable noisy optimization by branch-and-fit (SNOBFIT) which can solve the hidden constraints in a robust way have been developed [55]. It is necessary to develop a handling method because it is hard to consider the possibility of hidden constraint when forming surrogate with conventional regression model. Although several studies were performed with systematic optimization using explicit function of liquefaction process [56–59], explicit process modeling makes lots of works and complicated mathematical expression such as differential algebraic equation for kinetics can decrease the convergence rate. Conclusively, most compatible optimization algorithms for process modeling should need a global search algorithm, hidden constraints handling, robustness, and a consistent result. As can be seen in Table 1, typical algorithms that satisfy these properties are Lipschitzian-based partitioning techniques. Among these, DIRECT-type algorithm is an appropriate algorithm for solving general engineering problems [60–67]. It is proved by Jones and Finkel and Kelley [68,69] that if objective function is a deterministic and Lipschitzian continuous, then convergence to the global optimum is guaranteed. Since DIRECT does not require a Lipschitzian constant, there is no need to predict or compute it, so the parameter is actually only a Jones factor, and even this value has found an appropriate value [68]. Thus, deterministic and robust optimization can be performed. However, several improvements should be performed to apply DIRECT algorithm to the process optimization. DIRECT algorithm does not have a specific interpretation for handling hidden constraints [70]. Thus, if we want to integrate a derivative-free optimization scheme effectively with an unknown infeasible region with hidden constraints of the process simulator function, then we should develop an effective hidden constraint-handling algorithm. Therefore, in this study, we developed a sub-dividing step as a hidden constraint handling method to apply the DIRECT algorithm to process systems optimization. By applying this method to the SMR liquefaction process modeled by Aspen HYSYS, performance of the algorithm was validated.

The paper is organized as follows. A brief introduction about the original DIRECT method is described. The proposed modified DIRECT algorithm that has a sub-dividing step to handle hidden constraints is explained and compared with the previous methods of the barrier approach and neighborhood assignment strategy (NAS) [62]. To test the performance of the modified DIRECT algorithm with a sub-dividing step, a simple single mixed refrigerant (SMR) process for natural gas liquefaction with 3 hidden constraints modeled by Aspen HYSYS V8.8 is utilized. Finally, the optimized process is compared with the conventional DIRECT algorithms (barrier approach, neighborhood assignment strategy), the stochastic global search algorithms (GA, PSO, SA), the model based global search algorithm (SNOBFIT), and the several local search methods (GPS, GSS, MADS, SQP, active-set, interior-point).

2. DIRECT algorithm with hidden constraints

The DIRECT algorithm is based on Lipschitzian-based partitioning techniques and it can handle non-linear and non-convex functions globally [9]. Since many functions of process systems engineering in chemical engineering are calculated by commercial software assumed to be black-box models for users and as the equations are highly non-linear and non-convex, a deterministic derivative-free global optimization algorithm is appropriate. Moreover, after they evaluate the simulation, commercial process simulators give error messages because of convergence errors or a physically infeasible region. Thus, we should consider hidden constraints that do not give information of infeasibility before evaluating a function. In this research, we suggest a modified DIRECT algorithm to handle hidden constraints by using a sub-dividing step based on the original DIRECT algorithm.

2.1. Basic ideas of the original DIRECT algorithm

The mathematical description of the original DIRECT algorithm was developed by Jones et al. [68]. Two critical ideas were implemented in Shubert's algorithm for applying it to derivative-free optimization problems without the Lipschitz constant. First, hyper-rectangular partitions based on N-dimensional trisection are suggested. This can decrease the computational cost by evaluating the function at the center of the hyper-rectangle and not at all extreme points. Since the center point solution of the hyper-rectangle is conserved, unnecessary overlapped function calculations are not performed after partitioning. Second, the decision criteria regarding which hyper-rectangles should be divided are decided based on the concept of potentially optimal hyper-rectangles. At the iteration step, all hyper-rectangles are identified that are potentially optimal and only potentially optimal hyper-rectangles will be divided before passing to the next iteration. The brief description of the potentially optimal condition based on [68] is given in Definition 1.

Definition 1 Let i and j be the index of the hyper-rectangle and c_i and c_j be the center of hyper-rectangles i and j, respectively. d_j is a measure for this hyper-rectangle such as the distance from the center of hyper-rectangle i to its vertices. Let ε called Jones factor be a positive constant and let f_{min} be the minimum function value so far iteration. A hyper-rectangle j is called potentially optimal if positive $\tilde{K}$ exists such that

$$f(c_j) - \tilde{K}d_j \le f(c_i) - \tilde{K}d_i \quad \text{for } \forall i, \tag{1}$$

$$f(c_j) - \tilde{K}d_j \le f_{min} - \varepsilon|f_{min}|. \tag{2}$$

The step of identifying hyper-rectangles is performed at every iteration repeatedly. Thus, resolution of the searching area near the locally or globally optimal solution increases sequentially. A brief description of the DIRECT algorithm is shown in Algorithm 1.

Algorithm 1 DIRECT(upper and lower bound of variables, f, ε, termination criteria)

Normalize the searching space to be the unit hyper-rectangle.

Evaluate the function at the center of hyper-rectangle (c_1) and $f_{min}=f(c_1)$.

while termination conditions such as reaching the number of max iteration and function evaluation are activated

Identify which hyper-rectangles are the potentially optimal hyper-rectangles.

Divide all potentially optimal hyper-rectangles.

Evaluate the function value at the center of new hyper-rectangles.

Update $f_{min.}$

end while

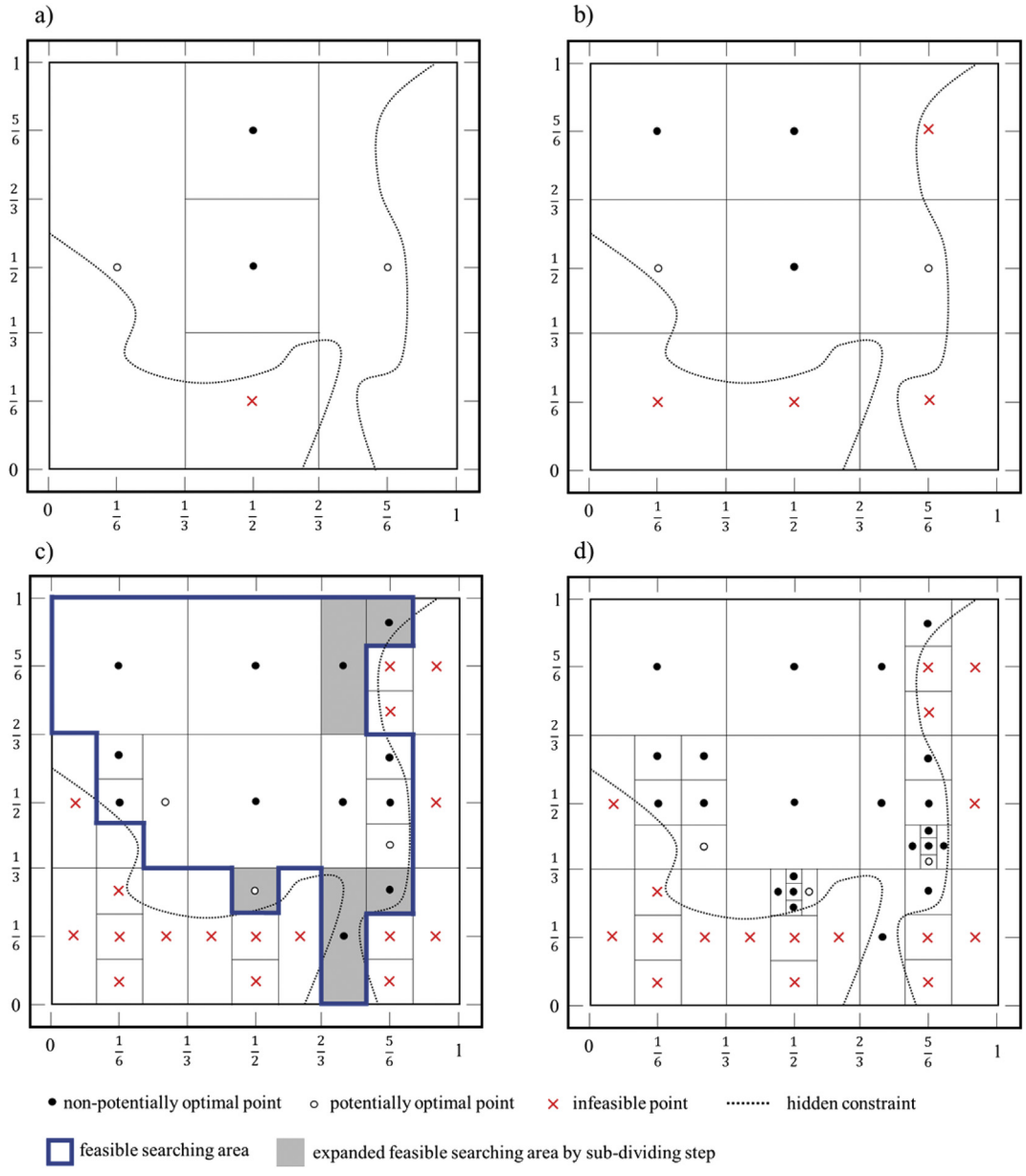

Fig. 1. Geometric interpretation of potentially optimal point and infeasible point using DIRECT with sub-dividing step algorithm on two dimension hidden constraints problem at a) the first iteration, b) the second iteration, c) the third iteration with the first sub-dividing step, d) the fourth iteration.

2.2. Modified DIRECT algorithm for hidden constraints

Generally, the DIRECT algorithm does not have a constraint-handling mechanism and its searching area consists of the upper and the lower bound of each variable. However, a constraint-handling mechanism should be needed to solve engineering application problems. Three constraint-handling methods were proposed which are the barrier approach, L1 penalty function [71], and the neighborhood assignment strategy (NAS) [62]. However, the L1 penalty function approach is not appropriate for hidden constraints because it requires a predefined explicit constraint. If a commercial process simulator diverges at an infeasible point, then it is impossible to use the L1 penalty function because it has no function value. Furthermore, although the barrier approach can handle the hidden constraint, it was not an appropriate method with DIRECT with hyper-rectangles with a large feasible area, but an infeasible center [72]. Thus, the function should be evaluated by checking whether the point is either in the hidden constraint or not and whether it can be effectively handled by NAS. NAS sets the enlarged rectangle whose center is an infeasible point and determines the surrogate value from the already evaluated feasible points. Thus, it does not need a penalty parameter or constraint function value. However, because NAS does not use information of constraints such as the shape of the constraint or constraint violations, its performance can decrease greatly when the shape of the constraints is highly non-convex [73].

To solve this problem, we suggest a sub-dividing step for infeasible hyper-rectangles that do not satisfy the hidden constraints. If the points are identified as infeasible points, then the function assigns a penalty value like the barrier approach. In the sub-dividing step, all infeasible hyper-rectangles are divided after dividing potentially optimal hyper-rectangles and the center values of the new hyper-rectangles generated by the sub-dividing step are calculated. After the sub-dividing step, new minimum function value is updated and goes back to the next iteration. A brief introduction of this algorithm is shown in Algorithm 2.

Algorithm 2 modified-DIRECT(upper and lower bound of variables, f, ε, termination criteria)

```
Normalize the searching space to be the unit hyper-rectangle.
Evaluate the function at the center of the hyper-rectangle (c1).
if f(c1) is feasible
        fmin=f(c1).
else
        Divide the first hyper-rectangle.
end if
while termination conditions such as reaching the number of max iterations and
function evaluations are activated
        Identify which hyper-rectangles are the potentially optimal hyper-rectangles.
        if sub-dividing step is activated
            Identify which hyper-rectangles have an infeasible function value
        end if
        Divide all potentially optimal hyper-rectangles
        Evaluate the function value at the center of the new hyper-rectangles.
        if sub-dividing step is activated
            Divide all infeasible hyper-rectangles
            Evaluate the function value at the center of the new hyper-rectangles.
        end if
        Update fmin
end while
```

To illustrate the sub-dividing algorithm, Fig. 1 shows a geometric graph of the DIRECT algorithm with a sub-dividing step at the third main iteration. Unlike the barrier approach, the sub-dividing step can decompose the edge of the hidden constraints and expand the feasible searching area. Thus, it is possible to consider complicated shape constraints with high skewness such as a non-convex shape. Although the calculation cost is higher than the original DIRECT algorithm because of the sub-dividing step, if sub-dividing steps are performed at the proper iteration, then performance can be increased effectively within computational limitations. For validating the performance of a simple problem with a hidden constraint, the Goldstein-Price test function, which is

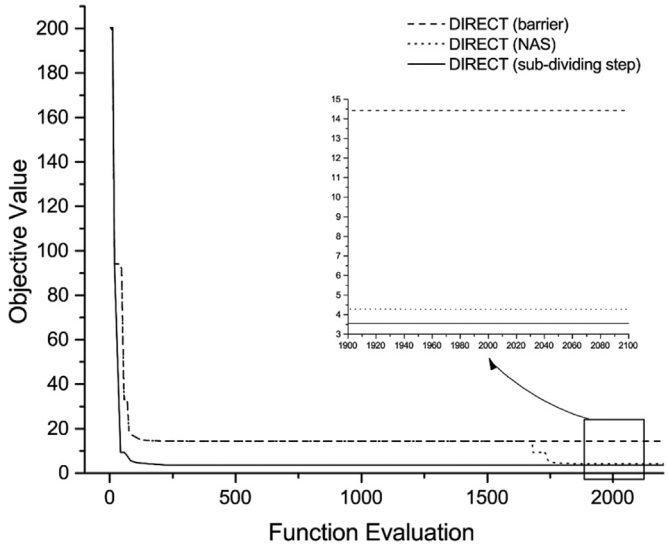

Fig. 2. DIRECT with barrier, NAS, and sub-dividing step iteration for Goldstein-Price test function.

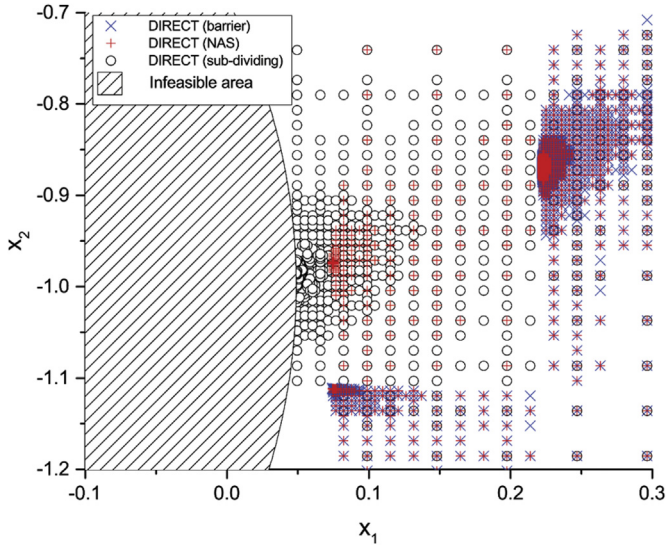

Fig. 3. The points where Goldstein-Price test function is evaluated with barrier, NAS, and sub-dividing step at 2000 function evaluation.

given by Eq. (3), is used [74].

$$\begin{aligned} f(x_1,x_2) = &\Big[1+(x_1+x_2+1)^2\big(19-14x_1+3x_1^2-14x_2 \\ &+6x_1x_2+3x_2^2\big)\Big]\Big[30+(2x_1-3x_2)^2\big(18-32x_1 \\ &+12x_1^2+48x_2-36x_1x_2+27x_2^2\big)\Big], \\ &\{x_1,\ x_2\}\subset D\cap D_{hidden} \end{aligned} \tag{3}$$

where the pre-defined feasible region D and hidden constraint D_{hidden} are defined as Eqs. (4) and (5).

$$D=\{(x_1,x_2)|(-2,-2)\le(x_1,x_2)\le(2,2)\} \tag{4}$$

$$\begin{aligned} D_{hidden}=\Big\{(x_1,x_2)|\Big[&(x_1+1)^2+(x_2+1)^2 \\ &\ge 1.1\Big]\cap\Big[(x_1-1)^2+(x_2-1)^2\ge 0.9\Big]\Big\} \end{aligned} \tag{5}$$

We assume that we do not know the value of D_{hidden}, thus only the function can determine that the point is feasible or infeasible and the optimization problem is $\min_{x_1,x_2\subset D\cap D_{hidden}} f(x_1,x_2)$. The sub-dividing step is activated at iterations 5 and 15. The barrier approach and NAS are also evaluated with a limited function evaluation number set to 2000 for comparing the algorithm performance in the same manner.

The objective function values versus function evaluation are illustrated in Fig. 2. Convergence speed of the barrier approach, NAS, and the sub-dividing step are similar at the early stage but the optimal values are different. The final optimal values are 14.4, 4.3, and 3.5, respectively. Moreover, NAS shows a second decreasing phase at about the 1700 function evaluation number point. It seems that NAS finds the feasible points in the enlarged rectangle with a surrogate model at that stage. In Fig. 3, the barrier approach and NAS show convergence values of feasible points at (0.22, −0.87) which is far from the infeasible circle hidden constraints while the sub-dividing step has convergent points at (0.049, −0.99) which is almost at the edge of the hidden constraints. Although NAS has a second set of convergent points at (0.074, −0.97), it is also farther from the hidden constraints than the sub-dividing step. The reason for inefficiency of the barrier approach is that the barrier approach deactivates the infeasible hyper-rectangle and that rectangle cannot be divided until optimization is over. Thus, the resolution of feasible rectangles near the hidden constraint is very low and we can see a rectangle barrier in Fig. 3. There is a possibility that NAS gives low performance when NAS fails to consider the shape of the hidden constraint and estimates the function value of an infeasible point from the surrogate model.

3. SMR liquefaction process for natural gas

The single mixed refrigerant (SMR) liquefaction process is one of the famous cryogenic mixed refrigerant processes because of its simplicity. The basic structure of the SMR process consists of a single stage cold box, a Joule-Thomson valve, and 4 series compressors with after-cooling. Although SMR processes are theoretically inefficient in exergy compared to advanced liquefaction processes, such as the dual mixed refrigerant (DMR) cycle and the propane pre-cooled mixed refrigerant (C3MR) cycle [57], they have been used because of their simple structure and network connections, which guarantee easy control, operation, and low capital cost. In this study, the base case of the SMR process was selected from Ref. [75] which consists of two multi-stream heat exchangers, a phase separator, three compressors, and after-cooling heat exchangers.

3.1. Process model and design variables

The process is modeled by Aspen HYSYS V8.8, which is a qualified commercial process simulator in the LNG industry. The process flow diagram and the name of each unit and stream are given in Fig. 4. Table 2 lists the simulation basis and feed conditions in the SMR process. The base operating condition and assumptions are provided from the literature and the readers should refer to [34]. The mixed refrigerant consists of nitrogen, methane, ethane, propane, and n-butane, and the composition of NG is nitrogen, methane, ethane, propane, i-butane, n-butane, and i-pentane. Peng-Robinson EOS is used for calculating thermodynamic properties. The production rate of NG and the minimum temperature

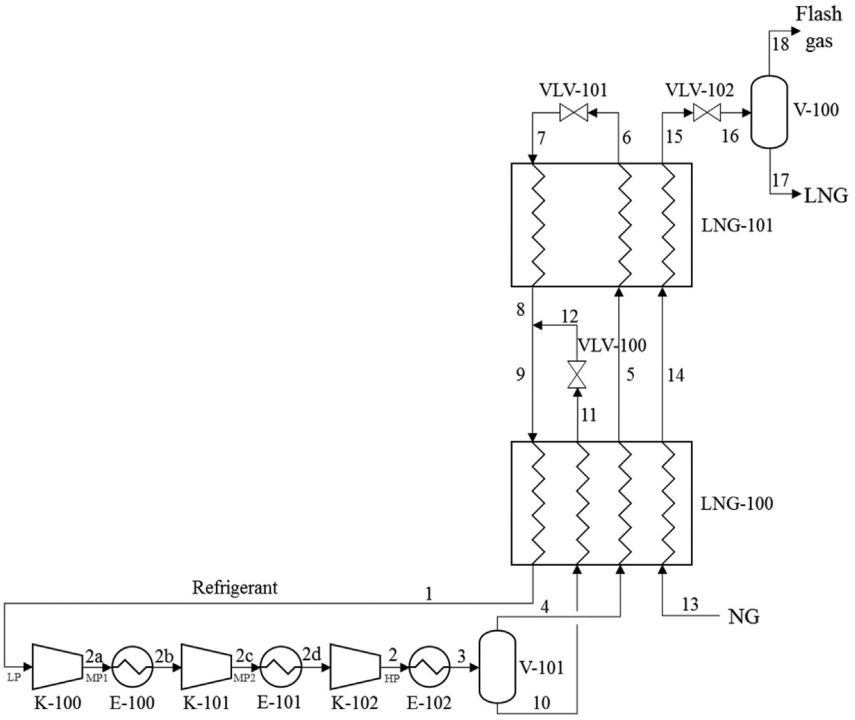

Fig. 4. Process flow diagram of single mixed refrigerant (SMR) natural gas liquefaction process.

Table 2
Base operating condition of SMR process and NG feed composition.

Property		State
NG feed		
Temperature (K)		300
Operating pressure (bar)		65
Flow rate (kg/h)		26.38
Composition (mol%)	Nitrogen	4.0
	Methane	87.5
	Ethane	5.5
	Propane	2.1
	i-Butane	0.3
	n-Butane	0.5
	i-Pentane	0.1
Minimum temperature approach at LNG-100 and LNG-101 (K)		2.85
Intercooler outlet temperature (K)		305
Compressor adiabatic efficiency (%)		80

Table 3
The lower and upper bounds of design variables.

Property	Lower bounds	Upper bounds
Pressure variables (bar)		
LP	0.300	5.700
MP1	0.750	14.250
MP2	1.875	35.625
HP	4.675	88.825
Composition variables (%)		
Nitrogen	0.859	16.321
Methane	2.597	49.343
Ethane	2.541	48.279
Propane	3.911	74.309
n-Butane	dependent	

approach (MTA) were fixed as 26.38 kg/h and 3±0.15 K, respectively. In fact, liquefaction process performance should be evaluated by not only exergy and compressor shaft work but also by capital cost. However, it is difficult to scalarize the operating cost and the capital cost in the same dimension such as cost. Thus, we bound MTA as ±5% of 3 K for keeping off the catastrophe, infinite area of the heat exchanger and set the minimum MTA of LNG-100 and LNG-101 of the base case as 2.85 K for comparison purposes. Centrifugal compression energy is calculated by the Schultz polytrophic method with 80% adiabatic efficiency. The pressure drop across the heat exchanger, flash drum, and mixer is ignored. Table 3 lists the 9 design variables, which are 4 types of pressure variables and 5 types of refrigerant composition, and their bounds. LP, MP1, MP2, and HP are the pressure of stream 1-start, 2a, 2c, and 2, respectively, which are connected to the compressors. Especially, LP is connected to the after stream of the Joule-Thomson valve, VLV-101, which directly affects exergy efficiency and the MTA of the cold box. Although LP can be changed to the temperature of stream 7 as in previous research [41], we selected this pressure variable for preserving the consistency of variable type. Although the mixed refrigerant is mixed with 5 pure chemical compounds, compositions of 4 of the compounds are enough to set the optimization problem because of the composition constraint, which limits the sum of composition equal to 100%. Previous researches [41,42] usually selected the bounds based on the preceding process knowledge, process designer experience, and sensitivity analysis of variables. However, that method is not efficient for the general purpose of optimization for various processes. Because the proposed optimization method can handle predefined constraints and hidden constraints simultaneously, the user does not need to find the nice bounds. In this research paper, the upper and lower bound of each variables are set to ±90% of the base set of the design variables.

For automating the connection between Aspen HYSYS V8.8 and the MATLAB optimization algorithm, the Aspen HYSYS SMR process case is set by objective function and ActiveX server communication technology is used and block diagram of combined algorithm and

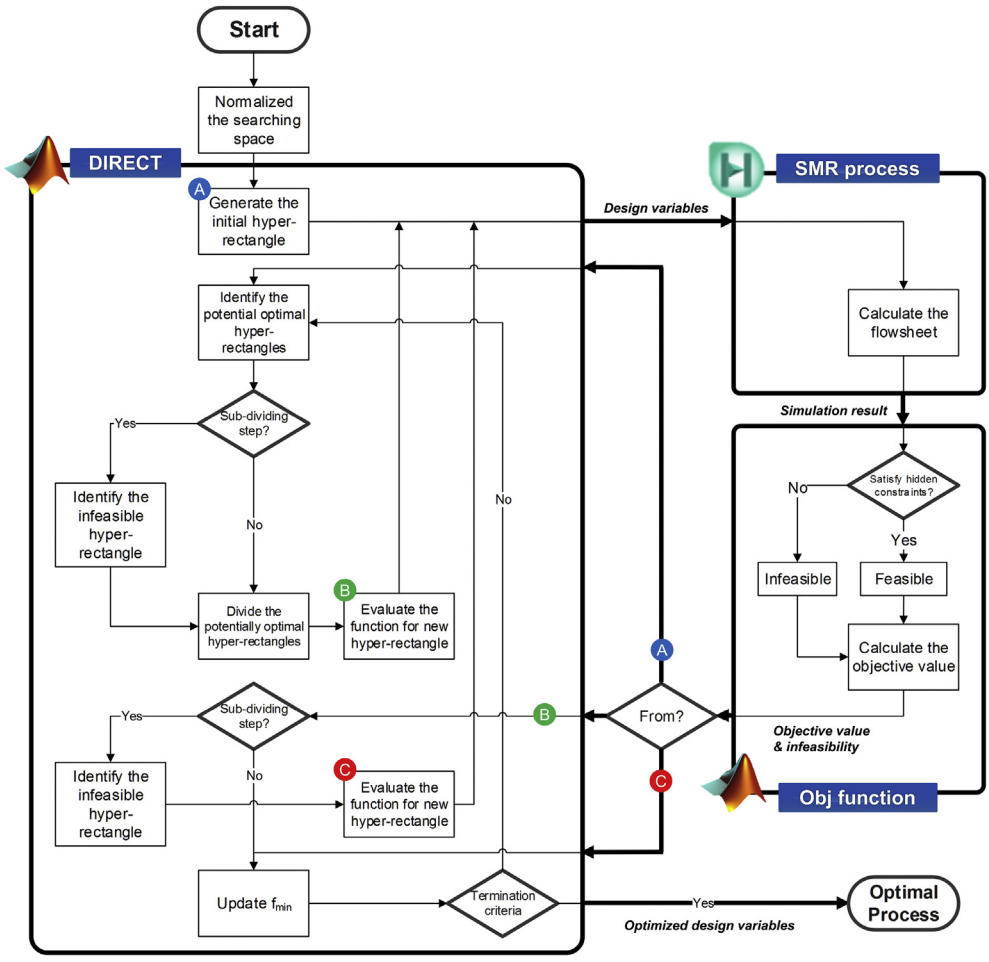

Fig. 5. Block flow diagram of optimization platform for DIRECT algorithm with sub-dividing step method for hidden constraint handling method and interconnection between optimization algorithm and Aspen HYSYS SMR process model.

process simulation function is shown in Fig. 5. Therefore, we can manage the process simulation as the function of MATLAB. Overall optimization algorithm is coded in the MATLAB and hidden constraints feasibility is also checked by external in-house code. Because of technical problems with the software, composition is changed by controlling the molar flow rate of pure component streams and the molar flow rate is determined by matching the temperature of 1-start and 1-end using the adjustment unit ADJ-1 with the secant method. Aspen HYSYS SMR process model, MATLAB-Aspen HYSYS ActiveX server interaction structure, and in-house objective function are provided at supplementary.

3.2. Optimization formulation

There are three types of constraints for process systems equations which are defined by the process simulator ($h_p(x)$), predefined constraints ($g_i(x)$, $h_j(x)$) and hidden constraints ($s_k(x)$). We should distinguish those constraints for different considerations. Brief optimization problem is given in (P).

$$\min_{x \in \mathbb{R}^{1\times n}} f(x) + \gamma p(x) \qquad \text{(P)}$$

subject to

$$g_i(x) \le 0 \quad i = 1,2,3$$

$$h_j(x) = 0 \quad j = 1$$

$$h_p(x) = 0 \quad p = 1,2,3,\ldots,m$$

$$p(x) = \begin{cases} 0 & \text{if } s_k(x) = 0 \text{ and } g_{i(x)} \le 0 \text{ and } h_j(x) = 0 \quad k = 1,2,3 \\ 1 & \text{if } s_k(x) \neq 0 \text{ or } g_{i(x)} > 0 \text{ or } h_j(x) \neq 0 \quad k = 1,2,3 \end{cases}$$

$$LB \le x \le UB$$

First, $h_p(x)$ such as the mass and heat balance equation, several thermodynamics equations, and other numerical equation systems are already defined by the process simulator. Thus, at the optimization platform, users do not need to consider those type equations precisely. Since the second type of constraints is predefined, it is possible to do not evaluate the function at out of constraints. Thus, if the variables set do not fit $g_i(x)$ and $h_j(x)$ which are linear constraints, a penalty function ($p(x)$) will be activated in the objective function and penalty parameter (γ) which is usually large value as barrier increases objective function. Thus, the process simulation function does not need to be evaluated. Predefined inequality constraints, $g_i(x)$, mean that the series connection of compressors should increase the pressure of each of the streams which is given

in (6). Predefined equality constraint, $h_j(x)$ means that the mole fraction (m_k) summation of overall chemical components mole fraction should be equal to 100% because of its definition (7).

$$P_{LP} \le P_{MP1} \le P_{MP2} \le P_{HP} \tag{6}$$

$$\sum m_k = 100\%, \quad k \in \text{all chemicals in SMR} \tag{7}$$

In this SMR process, there are three types of physically infeasible regions, which are 1) a case with no solution (divergent system), 2) a case with a temperature crossing point at LNG-100 and LNG-101, or MTA is not in 3±0.15 °C, and 3) a case that the liquid stream enters the compressors. However, it is impossible to know which design variable sets are in the infeasible regions before running the process simulator, which are also called hidden constraints. Thus, we judge this region as an infeasible hyper-rectangle for evaluating the process simulator function. With these three types of constraints, we integrated the process simulator with the modified DIRECT algorithm and the sub-dividing step using Aspen HYSYS and MATLAB. If the variable sets do not satisfy the pre-defined constraints and the hidden constraints, those points will be divided at the sub-dividing step. As in $g_i(x)$ and $h_j(x)$, $p(x)$ is activated and the penalty parameter is added to the objective function value. The objective function, $f(x)$ is the specific power required for NG liquefaction (kJ/kg-LNG) which is the total energy consumption of the compressor over the LNG product mass flow rate in stream 17. Since LNG should not be obtained as a multiphase form and vapor fraction of LNG must equal to 0, stream 17 after V-100 to measure the mass flow for liquid phase through flash calculation is selected.

For validating the performance of proposed algorithm, the algorithms given in Table 4 are tested. There are three types of stochastic global search algorithm, GA, PSO, and SA, which are the most famous nature-inspired metaheuristic algorithm. For fair comparison, population size for GA, swarm size for PSO, and reanneal interval for SA are set to 40. SNOBFIT is deterministic but model based search method and it has been known as robust and flexible for hidden constraints. GPS, GSS, and MADS are deterministic and direct search method but local search method based on pattern search. Finally, conventional constrained non-convex local optimization solver, active-set, interior-point, and SQP are tested with default option in MATLAB. In order to compare with the DIRECT algorithm under the same conditions, we tried to compare the values at the same computation cost based on the function evaluation. However, in the case of the local solver, the operation is stopped with the terminal criterion when the local optimum is lost and the operation is no longer meaningful. In the case of the DIRECT algorithm, barrier approach and the NAS for hidden constraint handling method are also calculated to compare the performance with the proposed method, the sub-dividing step. In order to compare the experiments under the same conditions, we try to compare the values at the same computation cost based on the function evaluation. However, in the case of the local solver, the operation is stopped with the terminal criterion when solver fall into the local optimum and the operation is no longer meaningful.

4. Optimization result and discussion

The optimization results of the SMR process are listed in Table 5. Since the objective function we have taken is the specific power required for NG liquefaction, results can be compared based on this value, and see how close the objective value approaches the constraint by looking at the MTA values of LNG-100 and LNG-101. For comparing each algorithm fairly, in the case of global search algorithm, the maximum number of iterations of the process simulator function is limited to 20,000 times. Meanwhile, the maximum number of iterations for local search algorithm is also limited to 20,000 times but all of them stop before it because of falling into the local optima. From the conclusion, the DIRECT algorithm with sub-dividing step successes in obtaining the most optimal value in the determined computation cost. This value is an energy saving effect of 18.9% for the base case, and 13% on average in comparison with other algorithms. Objective function value versus function evaluation of each algorithm is given in Fig. 6.

First of all, in case of DIRECT type solver, the specific power required for NG liquefaction from the sub-dividing step optimal solution is 1.7% and 9.2% lower DIRECT with the barrier approach, and NAS, respectively. Surprisingly, the result of the barrier approach is better than NAS. In Fig. 6, a graph of the barrier approach and NAS shows similar movement at the early stage; NAS cannot find a much better solution within the limited function evaluation whereas the barrier approach finds a better solution. It seems that the hidden constraint handling method of NAS is not appropriate for highly non-convex constraints or functions because its surrogate model assumes the neighborhood function value linearly, such as $F+\delta|F|$, where F is the low function value in the neighborhood around the infeasible center c. Since a physically feasible process, condition is very sensitive to design variables with non-convex hidden constraints, many populations and many iterations are needed to achieve a better solution. However, the solution fails when limited by the computational cost. Thus, the performance of NAS for an SMR process function is low and rather

Table 4
List of Algorithms for comparing the performance.

Solver	Global/Local	Deterministic/Stochastic	Constraints	Options
GA	Global	Stochastic	Yes	'Population Size' = {40} 'Crossover Fraction' = {0.5} 'Elite Count' = {2}
PSO	Global	Stochastic	Yes	'Swarm Size' = {40}
SA	Global	Stochastic	No	'Acceptance Fcn' = @modified_BoltzmannProbabilityDensity 'Reanneal Interval' = {40}
SNOBFIT	Global	Deterministic	Yes	Default
GPS	Local	Deterministic	Yes	'Poll Method' = 'GPS Positive Basis Np1' 'Search Method' = @GPSPositiveBasisNp1
GSS	Local	Deterministic	Yes	'Poll Method' = 'MADS Positive Basis Np1' 'Search Method' = @GSSPositiveBasisNp1
MADS	Local	Deterministic	Yes	'Poll Method' = 'MADS Positive Basis Np1' 'Search Method' = @ MADSPositiveBasisNp1
Active-set	Local	Deterministic	Yes	Default (fmincon option)
Interior-point	Local	Deterministic	Yes	
SQP	Local	Deterministic	Yes	

Table 5
Optimization result of SMR process.

Property		Base case	DIRECT sub-dividing step	DIRECT barrier	DIRECT NAS	GA	PSO	SA	SNOBFIT	GPS	GSS	MADS	Active-set	Interior-point	SQP
Total compression power (kW)		8.27	6.71	6.82	7.39	8.03	7.67	7.41	6.77	8.25	7.91	7.97	8.27	8.27	8.27
Specific power required for NG liquefaction (kJ/kg-LNG)		1170	949	965	1045	1136	1085	1048	958	1167	1118	1128	1170	1170	1170
Minimum temperature approach at LNG-100 (K)		3.01	3.00	3.02	3.00	3.05	3.00	2.99	3.00	3.01	3.00	3.00	3.01	3.01	3.01
Minimum temperature approach at LNG-101 (K)		2.85	2.85	2.96	3.27	2.87	2.93	3.53	2.88	2.85	2.88	2.85	2.85	2.85	2.85
Design variables															
Pressure (bar)	LP	3.12	3.87	3.07	3.00	3.58	2.87	4.39	5.70	3.12	3.44	3.41	3.12	3.12	3.12
	MP1	7.50	7.27	6.50	4.50	11.22	8.56	10.22	9.40	8.88	9.87	8.41	7.50	7.50	7.50
	MP2	18.75	13.10	9.17	7.50	24.35	19.82	17.08	16.07	22.75	23.26	17.88	18.75	18.75	18.75
	HP	46.75	28.05	24.93	18.70	47.15	37.99	39.85	38.32	46.75	47.10	47.32	46.75	46.75	46.75
Composition (mol%)	Nitrogen	8.59	8.58	7.83	8.59	8.91	6.93	11.25	11.93	8.59	8.68	8.63	8.59	8.59	8.59
	Methane	25.97	25.78	24.24	25.97	26.62	25.66	25.03	25.91	25.97	26.42	26.35	25.97	25.97	25.97
	Ethane	25.41	30.68	30.49	25.41	27.12	26.29	32.21	35.09	25.41	29.46	29.57	25.41	25.41	25.41
	Propane	39.11	15.64	15.64	15.64	34.21	34.40	19.03	10.47	39.11	29.86	30.11	39.11	39.11	39.11
	n-Butane	0.92	19.32	21.80	24.39	3.13	6.72	12.49	16.60	0.92	5.58	5.34	0.92	0.92	0.92
Computation cost (the number of process simulator function evaluation)		–	20,000							336	811	438	51	47	103

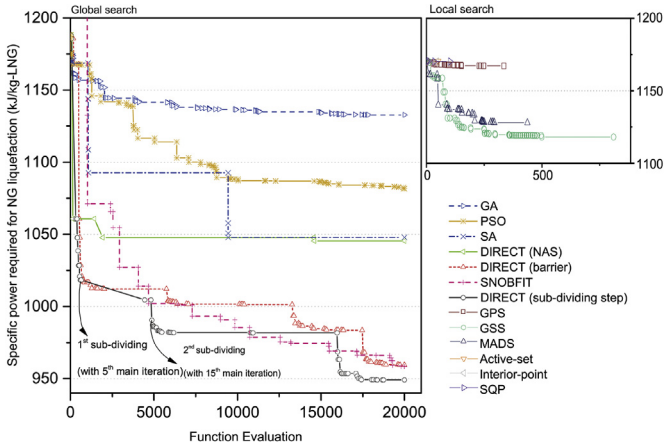

Fig. 6. Objective function value versus function evaluation of GA, DIRECT algorithm with barrier approach, NAS, and sub-dividing step.

the barrier approach and DIRECT with the sub-dividing step is better. Obviously, the sub-dividing step shows better performance than the barrier approach because sub-dividing step divide the edge of the hidden constraints and solution can approach closer to the edge.

In case of stochastic solver, GA, PSO, and SA, best found solutions are 16.4%, 12.5%, 9.4% higher than DIRECT with sub dividing step respectively. First, GA do not produce better results than expected. This seems to be due to the fact that the initial population selection has a great influence in the process of finding solutions. In the SMR process, the range of hidden constraints is quite wide, so if there is no initial procedure such as enumeration and the initial population is given randomly, there is a case where there is no feasible solution in the generation. This confirms the problem that most of calculations occur within an infeasible region even after significant generation. A total of 20,000 operations are performed five times and two initial population failure are detected. Among the others, the best performance trial is shown in Fig. 6. Although improved optimal solution can be found by changing various GA parameters such as crossover fraction, It is a disadvantage to do such additional operations. Similarly, in case of PSO, if all the swarms of the initial particles exist only in the infeasible region, the problem seems to occur because the direction or velocity of the particles cannot be calculated properly. However, unlike GA, 2 times are infeasible during 4 times, but 2 are better than GA. In case of giving several points which converged in DIRECT with initial swarm, it is about 4% better than DIRECT. However, this is another problem that determines what the initial swarm is given. Also, because there is a randomness tendency, it is not always possible to reproduce the solution in the same way. Therefore, it is can be said that the higher computation cost is needed. In case of SA, the Boltzmann probability density function, which is the default acceptance function, is used and since the penalty factor is increased, the temperature of the algorithm is drastically lowered and reannealing is prevented. Hence, we modify the algorithm to make the reannealing forcibly if the temperature is too low and continue the constant iteration at one point. The results show that SA shows similar performance to the DIRECT with NAS method. Overall, it seems that the stochastic solvers do not perform well in this optimization problem. Sometimes, however, solver can show nice solution with several trials because of their randomness characteristics and if initial procedure is well performed then solver can calculate the great solution. Despite probability of the great solution, it is impossible to guarantee that stochastic solver gives the best optimal solution deterministically. Thus, if the objective function is the case of high cost function, it is very inefficient and risky.

SNOBFIT, a deterministic and global solver, is a model based search method, but it is known to be an algorithm designed to handle hidden constraints very well. SNOBFIT gives the second best optimal solution following the DIRECT with sub-dividing step. However, because error between quadratic subproblem of SNOBFIT and original SMR process simulation function is relatively high up to about 5000 function evaluation, convergence rate is relatively slow than other algorithms. Even though SNOBFIT shows better optimal value at short interval, 12,000–16,000, DIRECT with sub-dividing step gives better optimal solution at the other intervals and has better early stage convergence speed.

Local solver gives a very bad solution overall. Even though the function evaluation is forced to 20,000, it fall into the local optimum, and the further operation became meaningless and stopped. Base case is given for initial point of local solver, which is the main factor of difference between the pattern search (GPS, GSS, MADS)

and conventional constrained non-convex solver (active-set, interior-point, SQP). Since the base case itself is precisely adjacent to the MTA hidden constraint (≥ 2.85 °C), if the LP rises even a little, the penalty function is activated because MTA of LNG-101 decreases. Because conventional constrained non-convex solvers change the main problem to the subproblem for handling the constraint effectively using the gradient information, they have tried to move through the gradient but they fail to find the better solution because of the discontinuity of hidden constraints. Thus, the final solutions of three solver are just same as base case. Unlike conventional constrained non-convex solvers, GPS, GSS, and MADS try to investigate the pattern of larger searching area and success to find better solution than base case. However, their solutions are 18.7%, 15.1%, and 15.9% higher than DIRECT with sub-dividing step respectively, which is terrible performance compared to global search algorithm. Herein, some reasons why solution might be considered as local optimum are explained. The results of the high-performance solvers in the global solver show that the n-butane content is significantly increased (more than 15%) and the HP pressure is significantly reduced (less than 40 bar) compared to the base case, which decrease the compressor power. However, if the change is continuously simulated on the simulator, it is impossible to converge continuously which means there are some discontinuous hidden constraints. In the case of the local solvers, they fails to pass the hidden constraints barrier during iteration and stops.

The optimal design of an SMR process has lower HP pressure and propane composition and higher n-butane composition than the base case. In fact, the process simulator convergence of LNG-100 and LNG-101 highly depends on the composition of refrigerant, LP, and HP. Thus, the DIRECT with hidden constraint handling method can the point to where low HP pressure decreases the total compressor work ensuring convergence by changing the refrigerant composition. In Fig. 7, the hot and cold composite curve of LNG-100 and LNG-101 shows that the composite curve of the optimal case from DIRECT with the sub-dividing step adjoin closer to each other than the base case. Thus, we can conclude that exergy efficiency, which represents the efficiency of the overall liquefaction process, of the optimal case is better than the base case. Furthermore, in Fig. 8, the overall ΔT profile of the optimal case is lower on average than the base case and the maximum ΔT of the optimal case is 24.8 K while the base case is 46.9 K. Thus, although the minimum temperature approach of the two cases is the same, the optimal solution can have high efficiency. Finally, the heat exchanger separation line, which is the discrete heat flow line between LNG-100 and LNG-101, moves to the right in the optimal solution. The overall heat flow quantity of the optimal solution increases and most of that quantity is allocated to LNG-100 because the ΔT profile of LNG-100 is better than for LNG-101.

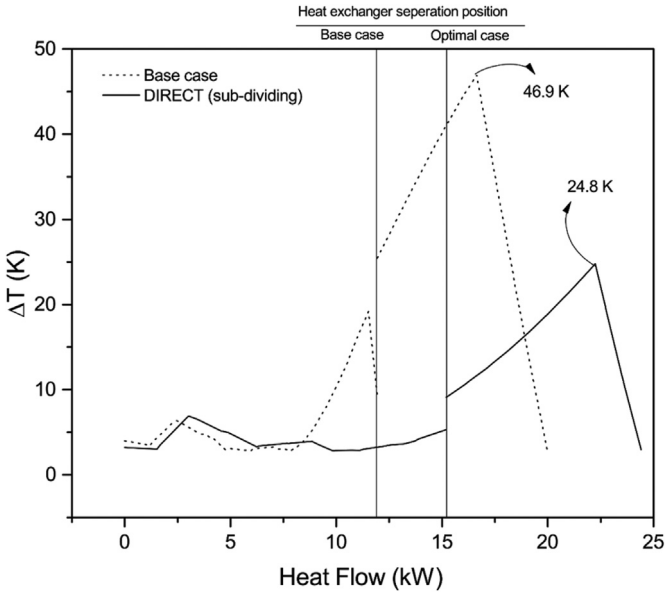

Fig. 8. ΔT profile in the cold box of base case optimal and DIRECT algorithm with sub-dividing step.

5. Conclusion

The modified DIRECT algorithm using sub-dividing steps is suggested as a means to handle hidden constraints. Unlike conventional methods such as the barrier approach and NAS, the sub-dividing step method can consider non-convex shape hidden constraints efficiently by partitioning the edge of the constraints. Thus, the DIRECT algorithm can search an expanded feasible searching area better than other methods. The DIRECT with sub-dividing step optimization decreases HP and increases n-butane content for lower compression specific power demands compared to the base case. To illustrate, the SMR NG liquefaction process with a commercial process simulator is optimized and provided a 18.9%

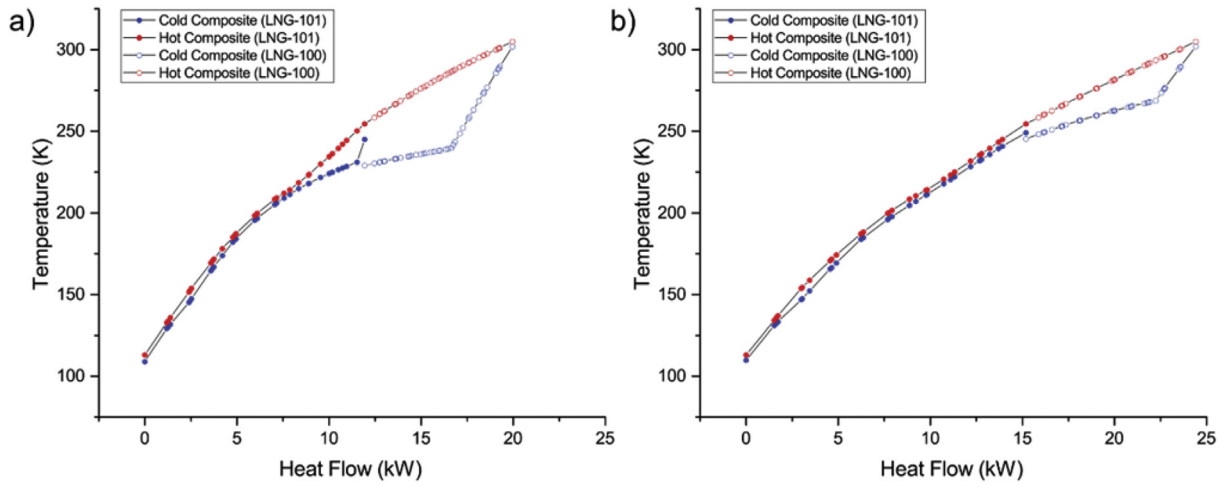

Fig. 7. Hot and cold composite curve of a) base case and b) optimal solution of DIRECT algorithm with sub-dividing step.

better solution than the base case. In comparison with GA, PSO and SA, the proposed algorithm solves the problems of reproducibility and initial procedure of stochastic solver based on deterministic characteristics and efficiency of algorithm itself and DIRECT with sub dividing step provides 16.4%, 12.5%, 9.4% better solution respectively. The result is even 1.7% and 9.2% better than the DIRECT algorithm with other hidden constraint handling methods, the barrier approach and NAS, respectively. We strongly believe that the proposed algorithm has advantages for optimizing chemical processes, not only SMR process, but also many processes developed in a commercial simulator such as the Aspen HYSYS because of its non-linearity and non-convexity with a large hidden constraints area. However, significant improvements on the original DIRECT algorithm and DIRECT with a sub-dividing step are required for a numerically robust and reliable solution. The proposed methodology cannot guarantee that which iterations are the best for the sub-dividing step. Moreover, not all infeasible hyper-rectangles but rather selected hyper-rectangles located in the edge of the hidden constraints should decrease the computation cost. Finally, if the DIRECT algorithm is modified for considering integer variables, then it can be applied for mixed integer non-linear programming (MINLP) problems such as mixed refrigerant selection, superstructure optimization of process design, and heat exchanger network synthesis (HENS).

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.energy.2017.03.047.

Nomenclature

ALAMO	algebraic models for optimization
c	center of hyper-rectangle
C3MR	propane precooled mixed refrigerant
d	measure for hyper-rectangle
D	predefined constraints
D_{hidden}	hidden constraints
DIRECT	Divide a hyper-RECTangle
DMR	dual mixed refrigerant
GA	genetic algorithm
GPS	generalized pattern search
GSS	generating set search
HENS	heat exchanger network synthesis
HP	high pressure
i	index of hyper-rectangle
j	index of hyper-rectangle
k	index of chemicals
$\tilde{K}$	potential optimal index
LNG	liquefied natural gas
LP	low pressure
m	mole fraction in percentage
MADS	mesh adaptive direct search
MINLP	mixed integer non-linear programming
MP	middle pressure
MTA	minimum temperature approach
NAS	neighborhood assignment strategy
NG	natural gas
ORC	organic Rankine cycle
PSO	particle swarm optimization
RSMs	response surface methods
SA	simulated annealing
SMR	single mixed refrigerant
SNOBFIT	Stable Noisy Optimization by Branch and Fit
γ	penalty factor
δ	positive constant for NAS
ε	Jones factor

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