Application of Surrogate-Assisted Gray Wolf Optimization (SAGWO) Algorithm for Optimization of Large-Scale Process Plants with Computationally Expensive Evaluation – Gas to Liquids (GTL) Process Case Study

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Abstract
Process optimization is necessary in order to decrease energy consumption and production costs. Using surrogate models, rather than mathematical modeling or simulator software, is an effective method to decrease the calculations and the time needed for optimization. Developing an offline data-based surrogate model for the whole response space requires generating a big data set. This itself involves numerous calculations and, therefore, would be too time-consuming. In this paper, the utilization of an online optimization algorithm is addressed for large-scale processes with a high computational burden. In this algorithm, by using of Latin hypercube sampling (LHS) method and the grey wolf meta-heuristic optimization algorithm (GWO) in combination with the support vector machine (SVM), a suitable balance between exploration and exploitation abilities is achieved. For comparison, the value of the objective function in the estimated global optimum point (GOP) and the number of objective function evaluations (NFEs) required to converge to GOP are investigated. The large-scale gas to liquids (GTL) process plant is chosen as a case study. The results showed that in the online method, while decreasing NFEs to less than one-tenth of the offline method, the GOP is found with a relative error of 0.1 percent.

Keywords: Process optimization, Grey wolf optimization (GWO), Gas to liquids (GTL)

Introduction
Optimization is the use of numerical or analytical methods to find the extremum of an objective function. Numerous examples in different fields of process engineering that require optimization are abundant. However, due to various reasons, including the nonlinear nature of processes, the complexity of response space and the difficulty, or inaccessibility to analytical modeling, the implementation of optimization may be highly challenging. The extent of such problems is even more for large-scale process plants. Existence of more complicated thermal and mass integrations, recycles, more operational constraints, more complex equipment like towers which require convergence of a set of specs, reactors, and the interactions between them are instances of such challenges.

During the last two decades, optimization methods based on evolutionary computation and swarm intelligence have been popular among researchers of artificial intelligence and soft computing [1, 2]. However, these methods are often ineffective due to their high computational complexity and the requirement of multiple evaluations of the objective function [3-5].

The use of process simulators like Aspen Plus and Aspen HYSYS as a replacement to analytical modeling to investigate the performance of chemical processes is a conventional procedure. One of the major problems in using these simulators in the optimization of large-scale processes is that the convergence of the simulation in a new conditions is very time-consuming and computationally expensive.

One of the useful ways to face these challenges is using surrogate models [6]. Ordinarily, surrogate models are used instead of process simulations, which leads to a significant decrease in the required time for optimization [7, 8]. Overall, there are two ways to utilize surrogate models in process optimization. The first way is the offline method [9-11], which provides a surrogate model of a process using a pre-prepared data set that is well spread in response space. On this premise, optimization will be executed on a trained surrogate model without another evaluation of objective function. However, it should be noted that the use of the offline method has an inevitable problem. The development of an accurate and reliable surrogate model of response space using a small data set is impossible. It will be more complicated when the high modality and complexity of response space accompanied by large dimensions. In this regard, the development of a large data set is necessary. This increases the amount of calculations and makes the problem even bigger.

In the online method [12-16], firstly, a simple model of response space based on an intelligent sampling method is created. After that, in every execution of the algorithm, some specific points of response space are added to the data set. Thus, gradually more accurate model is trained in more important areas.

The desired results of various online methods are reported in the literature. Liu et al. [17] developed a surrogate-assisted evolutionary algorithm based on the Gaussian process, which can optimize 20 to 50 dimensions problems. Regis [18] defined an RBF-based optimization algorithm that used PSO meta-heuristic algorithm for 30 to 36 dimensions problems. Sun et al. [19] presented a surrogate-assisted optimization algorithm based on swarm cooperation, which is benefited from PSO in social learning. Wang et al. [20] developed a novel evolutionary sampling assisted optimization method so that acceptable results are achieved on 20 to 200 dimensions test functions by using local and global surrogate models.

In this paper, the natural gas to liquids (GTL) large-scale process plant is investigated as a case study. The results of the GTL process optimization using its Aspen HYSYS simulation are reported in [21] and [22]. Because the GTL process unit contains recycles, adjustments, and several chemical reactors, each time of simulation run has a high calculation load and therefore takes a long time. To overcome this issue, application of surrogate models for process optimization in an offline way is investigated in [23].

In this study, an online method is used to optimize the GTL process, and finally, the results are compared with the results reported by other references. For this purpose, the surrogate-assisted grey wolf optimization (SAGWO) algorithm, which is provided in [24], was used accompanied by a support vector machine (SVM) as a surrogate model. This algorithm evaluates a limited number of points in the response space with a specific strategy. Therefore, in addition to exploiting the previous findings, try to explore more potential areas, and extract the most possible knowledge from a limited number of evaluations.

Experimental

The support vector machine (SVM) provided by Vapnik in 1995 [25] was considered a well-known and intelligent computational method in regression and classification. This method has a high potential in nonlinear fitting and has shown an acceptable performance for small data sets [26].

The gray wolf optimization (GWO) algorithm is a meta-heuristic algorithm inspired by the hierarchical structure and social behavior of gray wolves during the hunting. This algorithm is population-based and can readily be extended to solve large-scale problems. It has three basic steps. First is watching the hunt, following and tracking it. Second is approaching and surrounding until it stops moving and finally is attacking. What happens, in reality, is that the direction of all the gray wolves is determined by the hunt location. The hunt in mathematical modeling of this algorithm is equivalent to the global optimum point of the response space. At the start of the optimization, when there is no information about the global optimum point location, the location of three major classes of wolves -Alpha, Beta, and Delta- is used.

In gray wolf optimization, after each iteration, the most favorable solution is considered as Alpha, and then the second and third best solutions will be named Beta and Delta, respectively. All the other answers are considered as Omegas, and their positions will be updated in relation to Alpha, Beta, and Delta. The provided algorithm in [24] is a GWO optimization algorithm based on a radial basis function (RBF) neural network that, in an online approach, optimizes the objective function. This algorithm includes three interrelated phases.

In the first stage, an initial population is distributed intelligently in the response space by the Latin hypercube sampling (LHS) method. In this distribution, a large portion of the response spaces is seen by the minimum number of points, and the initial evaluation is done effectively. In the second phase utilizing the RBF surrogate model, an estimation of the location of the possible global optimum point is created and evaluated by the objective function. This exploration is general and considers the whole response space.

In the third phase, two steps of local search, first by GWO and the second by a local optimization algorithm such as sequential quadratic programming (SQP), are done. The possible locations for the optimum point are determined and searched once by the global optimization algorithm and again from several various starting points by a local optimization algorithm. The estimated optimum points are finally evaluated by the objective function as well. Therefore, this algorithm consists of several steps of searching and potentially can collect the most information from the response space by the lowest number of objective function evaluations and move toward the global optimum point. In this paper, the SVM surrogate model is used instead of the RBF neural network. The flowchart of this algorithm is presented in Figure 1.

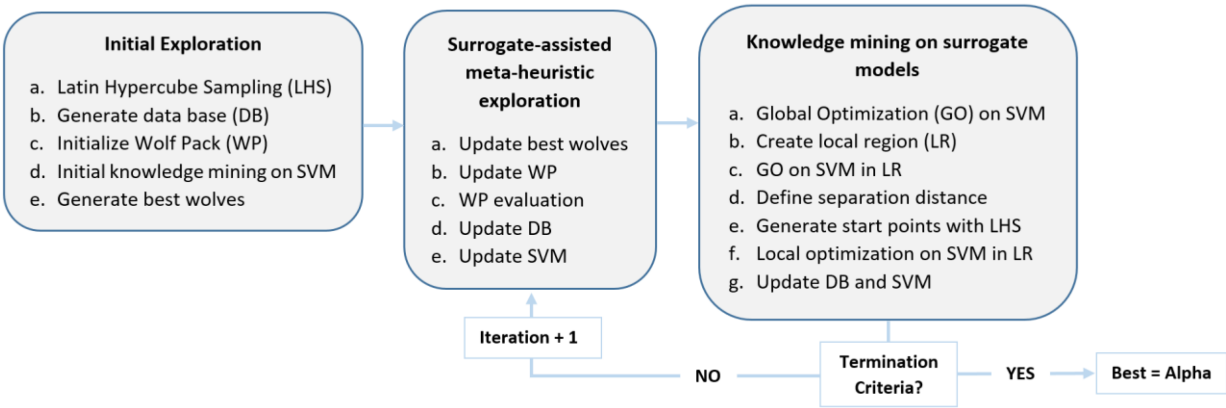

Figure 1 Simple flowchart of SAGWO algorithm [24]

Results and discussion

To optimize the GTL process, the production rate of wax in the process is defined as the objective function that should be maximized in this case. The optimization variables and their lower/upper bounds are given in problem 1 [21].

$$\begin{aligned}
&\boldsymbol{Maximize_{x_i}\ wax\ production\ \left(\frac{kg}{h}\right) Where}\\
&\boldsymbol{0.32 \le x_1: CO_2\ removal\ percentage \le 0.8}\\
&\boldsymbol{0.4 \le x_2: \frac{H_2O}{C}\ entering\ the\ syngas\ section \le 0.8}\\
&\boldsymbol{0.55 \le x_3: Recycled\ tail\ gas\ to\ FT\ ratio \le 0.8}
\end{aligned} \tag{1}$$

The optimization of this process is done by Panahi et al. using the optimizer plugin of Aspen HYSYS software, and the results are reported in [21] and [22]. Besides, the results of GTL process optimization, which is done by the MLP-GA combinatorial algorithm as an offline surrogate-assisted method, are reported by Khezri et al. in [23].

The abovementioned results are presented in Table 1.

Table 1 Reported results of GTL optimization in [21-23]

	CO_2 removal	H_2O/C	Recycle to FT	wax production (kg/h)
Ref. [21, 22]	0.32	0.4	0.61	77753
Ref. [23]	0.32	0.4	0.7	77860

The result of the GTL process optimization using the MLP-GA method in [23] is achieved with 420 NFEs. Also, this optimization is executed for two other cases of 16 and 81 data points in [23]. The results of which are reported in Table 2.

Table 2 Optimization results with various NFEs in [23]

	Num. of Points	wax production (kg/h)
MLP 1	420	77860
MLP 2	81	74821
MLP 3	16	73040

In this regard, the SAGWO algorithm has to provide similar results in a lower number of NFEs than the MLP-GA, or in an equal number of NFEs, it should search a higher wax production rate in the response space. To analyze this, the SAGWO algorithm was applied on the GTL process plant in two different cases. First with 16 NFEs and the next with 41 NFEs. The results of these two optimization cases are shown in Table 3.

Table 2 Results of GTL optimization with SAGWO algorithm

NFEs	CO_2 Removal	H_2O/C	Recycle to FT	wax production (kg/h)
41	0.32	0.40	0.635	77769
16	0.33	0.48	0.749	76966

A slight difference between the wax production rate with 41 NFEs by using SAGWO in table 3, and the GOP related to MLP 1 in table 2 with 420 NFEs, evidently shows the strength of SAWGO algorithm. Additionally, in the case with 16 NFEs in table 3, the algorithm is converged to a local optimum point in which the amount of produced wax is considerable and has a meaningful difference with 16 and 81 NFEs cases in table 2.

Conclusions

The optimization of large-scale process plants, which requires extensive computation, needs the development of more innovative and intelligent algorithms. The competing MLP-GA approach provides superior results when compared to the conventional method of process optimization using the simulator software's plugin. But it needs a big pre-prepared data set for execution, which itself is computationally expensive and time-consuming. Therefore, it does not appear to be an effective method to overcome main challenges, which are saving of time and process load. In this study, by analyzing and compiling the SAGWO algorithm to optimize the GTL process plant, a comparison is made between achieved results in the present work and the results reported in two other articles. This comparison shows a substantial reduction in calculation load to one-tenth while keeping the accuracy and converging to the global optimum point. In other words, by using the SAGWO method with 41 NFEs, it is possible to achieve the same results, which are gained by 420 NFEs in the MLP-GA method. This considerable reduction clearly shows that, if the intelligence is used correctly in the optimization procedure, better results are achievable with lower cost.

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