



A modified optimization method for optimal control problems of continuous stirred tank reactor

Mitra Salimi^{a,*}, Akbar H. Borzabadi^b, Hamed H. Mehne^c, Aghileh Heydari^a

^aDepartment of Mathematics, Payame Noor University, Tehran, P.O. Box. 19395-3697, Iran

^bDepartment of Applied Mathematics, University of Science and Technology of Mazandaran, Behshahr, Iran

^cDepartment of Avionics, Aerospace Research Institute, Tehran, 14665-834, Iran

(Communicated by Madjid Eshaghi Gordji)

Abstract

Continuous stirred tank reactor (CSTR) is an important and constructive part in various chemical and process industries and therefore it is necessary to control the process in optimal temperature and concentration conditions. Because of the nonlinear nature and limits of the control input, solving this problem is very difficult. To achieve a sub-optimal control policy for chemical processes, we focused on a new construction model. Then, a two-phase algorithm, denoted as modified sequential general variable neighborhood search (MSGVNS) algorithm based on three local searches that use efficient neighborhood interchange has been employed to solve CSTR problems numerically. The results of the proposed method show that its convergence to the exact solution is achieved by the accuracy comparable to other numerical algorithms in few times.

Keywords: Optimal control problem, Metaheuristic, Continuous stirred tank reactor, Modified general variable neighborhood search

2010 MSC: Primary 90C33; Secondary 26B25.

1. Introduction

CSTR is a common reactor in chemical process for efficient mixing. It was widely used in industrial applications [1, 2, 3], pharmaceuticals [4], and wastewater treatment units [5]. The need to keep its temperature and concentration of outputs at prescribed levels motivates researchers to derive its mathematical model. The combination of chemical reactions and phase equilibrium makes the CSTR

*Corresponding author

Email addresses: salimi2012a@gmail.com (Mitra Salimi), akbar.h.borzabadi@gmail.com (Akbar H. Borzabadi), hmehe@ari.ac.ir (Hamed H. Mehne), a-heidari@pnu.ac.ir (Aghileh Heydari)

Received: 19 July 2020 *Revised:* 23 September 2020

model complex and nonlinear with both stable and oscillatory behavior. As examples of studying the dynamics of CSTR we may refer to [6] where, the feasible solutions of CSTR were obtained using the homotopy perturbation method, and the effect of CSTR parameters on its stability was studied by [7]. If minimum energy for control environmental parameters is desired, CSTR will be the plant in an openloop control problem. Therefore, the optimal control of CSTR has appeared in several research works. For example, in [8] the estimation of optimal control for CSTR was obtained using model predictive control and extended Kalman filter, the continuous genetic algorithm was implemented by [9] to find the optimal solution of CSTR as a benchmark problem, maximum principle and phase plane analysis were used to solve the time-optimal control problem for a CSTR by [10], and the CSTR was utilized as a test case by [11] to examine the efficiency of a numerical method for optimal control problems. In this paper, the solution of different CSTR with single, two, and more phases of the reactor is discussed. To solve the problem with the help of metaheuristics, the CSTR is turned first into a finite large dimensional nonlinear programming (NLP) problem by discretizing the space-time and control. Then, an efficient metaheuristic method is extended to solve the problem in a reasonable time. The optimization problem of assignment in time-control space is considered as a hub location problem. This enables us to bring up two-phase modified sequential general variable neighborhood search (MSGVNS) as an outstanding method for hub location problems. It is expected that the design of this algorithm based on structural similarity will have many benefits, including its programming is very easy, it solves a wide range of problems, the calculation time is very short, the initial approximation is very close to the optimal solution and it is absorbed to a minimum globally, which leads to improved CSTR solutions. The remainder of this paper is organized as follows: In Section 2, the CSTR formulation, its analysis, and discretization are explained. In Section 3, two-phase MSGVNS is described and gives a detailed analysis of the proposed algorithm. In Section 4, we present several examples of CSTR. Finally, Section 5 summarizes the main conclusions of our research for CSTR.

2. Mathematical programming formulation

CSTR suggested in the handbook of the test problem in local and global optimization subject is benchmark problem [12]. The standard CSTR model is a set of two nonlinear differential equations obtained from dynamic equilibrium materials and energy:

$$V c_p \rho \frac{dT_R}{d\theta} = q c_p \rho (T_0 - T_R) - V U^* + (-\Delta H) V R, \quad (2.1)$$

$$V \frac{dc_A}{d\theta} = q(c_{A_0} - c_A) - V R, \quad (2.2)$$

where:

- c_A ($kmol.m^{-3}$) is the concentration of species A leaving reactor.
- c_{A_0} ($kmol.m^{-3}$) is the concentration of species A in feed stream.
- T_R (K) is the temperature of reactants leaving reactor.
- T_0 (K) is the temperature of feed stream to reactor.
- θ (min) is time.
- V (m^3) is the volume of reactor.
- R ($mol.m^{-3}.min^{-1}$) is the reaction rate term.
- q is the volumetric flow rate of feed and output streams.
- $-\Delta H$ ($kJ.mol^{-1}$) is the heat of reaction.
- c_p ($kJ.kg^{-1}.K^{-1}$) is the heat capacity of reacting mixture.

- $\rho(kg.m^{-3})$ is density of reacting mixture.
- $U^*(kJ.m^{-3}.min^{-1})$ is heat transfer term corresponding to cooling coil in reactor.

According to [13], (2.1) - (2.2), when CSTR is used in a stable state, mathematical explanations are minimized:

$$J(x(\cdot), u(\cdot)) = \int_{t_0}^{t_f} g(t, x(t), u(t))dt, \tag{2.3}$$

where, $x(t) \in \mathbb{R}^r$ is the state function, $u(t) \in \mathbb{R}^s$ is the control function, and J is the performance index. The control and state functions are respectively input and response of the following dynamical system, constraints and initial conditions:

$$\dot{x} = f(t, x(t), u(t)), \tag{2.4}$$

$$x(t_0) = x_0, x(t_f) = x_{t_f}, \tag{2.5}$$

$$u_l \leq u \leq u_b, \tag{2.6}$$

where $f : \mathbb{R}^r \times \mathbb{R}^s \times \mathbb{R} \rightarrow \mathbb{R}^r$, $g : \mathbb{R}^r \times \mathbb{R}^s \times \mathbb{R} \rightarrow \mathbb{R}$ are sufficiently smooth on suitable open sets. u_l and u_b are s -dimensional constant vectors that determine the lower and upper bounds for the control function.

2.1. CSTR as p -Hub median problem

For performing MSGVNS to solve CSTR, we focus on transform to p -HMP (see [14] for more details). In HLP, traffic between two nodes is not done directly, but through a specific set of nodes, known as the hub. Hubs are nodes that support and distribute the current in a specific set of nodes for transportation and communication systems with many demands and assigning the non-hub nodes to the selected hubs. Many expensive direct connections (origin-destination) can be eliminated and the transport flow can be made more efficient.

There are many types of HLP. For example, it may be assumed that the exact p hubs should be chosen, which is called p -HMP. The p -HMP focuses on the location of the hubs and the allocation of non-hub nodes to these established hubs to minimize total transportation costs (time, distance, etc.). Under a single allocation (SA), all-time nodes are assigned to a single control as hub [15]. Additional changes include limited capacity (capacitive) or unlimited (uncapacitated) capacity at the hub (USApHMP). A comprehensive review of available methods and solutions can be found in [16, 17].

For this, the time interval is uniformly divided by using a constant number of time nodes, then the control variable is approximated by a scalar matrix of control input values. So, we try to find optimal or sub-optimal results for the discretized formulations to approximate the global solutions of CSTR. The first step is to discretize the problem of minimizing (2.3) subject to (2.4)-(2.6). Fir this, $[t_0, t_f]$ divided to n subintervals as follow:

$$[t_0, t_1], [t_1, t_2], \dots, [t_{n-1}, t_n = t_f]. \tag{2.7}$$

To get optimal control for the problem (2.3)-(2.6), can focus on finding an optimal piecewise linear control function $u(\cdot)$ on each time sub interval. Corresponding each interval $[t_{i-1}, t_i], i = 1, 2, \dots, n$, partition the interval $[u_l, u_b]$ is partitioned to m equal sub intervals $[u_{j-1}, u_j], j = 1, 2, \dots, m$ that $u_0 = u_l$ and $u_m = u_b$. In the following, p constants u_1, \dots, u_p from m sub interval are selected.

$$\{t_0, t_1, \dots\} \rightarrow \{u_0, u_1, \dots\}, \tag{2.8}$$

An optimization problem with a finite number of decision variables is produced indicating that the assignment of a controller should not be limited for each time selection and output capacity, so we have USApHMP.

2.1.1. Evaluation

For discretization, piecewise linear control function with its values as input for the main continuous problem is constructed as:

$$u(t) = \sum_{k=1}^n \xi[t_{k-1}, t_k](t) u_k. \quad (2.9)$$

In fact, using the characteristic function:

$$\xi[t_{k-1}, t_k](t) = \begin{cases} 1, & t \in [t_{k-1}, t_k] \\ 0, & \text{otherwise} \end{cases} \quad (2.10)$$

Variables $\xi[t_{k-1}, t_k]$, serving as hub indicators, are restricted to be 0 or 1. In (2.3), the term integral can be estimated by a numerical method of integration and $X = [x_1, x_2, \dots, x_n]$, can approximately be computed by the newton or forth Runge-Kutta methods. By discretization of the NOCP, the problem is changed to an optimization problem with an extra objective function.

Let

$$t_j = t_0 + jh, j = 1, \dots, n, \quad (2.11)$$

be time nodes, where t_0, t_f are the initial and final times, respectively.

The performance index (2.3) by numerical method finds the following discrete format as follows:

$$\text{minimize } J = \sum_{j=0}^n w_j g(t_j, x_j, u_j), \quad (2.12)$$

where, $w_j, j = 0, \dots, n$ are suitable arbitrary constants. Now, the reduced problem is minimizing (2.12). The optimum values of u_0, u_1, \dots, u_m determine the solution of the problem approximately based on (2.9).

Each assignment is represented with an array of length $n + p$ and consists of two segments. The numbers of hubs in this assignment are p , and for $1 \leq i \leq n$, location i is allocated to hub $h[i]$. Let us for each hub i in USApHMP $h[i] = u[j]$, $1 \leq j \leq m$, where j is the partition of control function and every time is assignment to one hub. Figure 1 (a), typical discretization with $n = 7$ and $m = 6$, is shown where time intervals assigned to each chosen pattern and so the best performance index is determined to find the near-optimal control of the problem. Figure 1 (b), is an example including the set of all hub and location assignments in NOCP with $n = 7, m = 6$ and $p = 5$.

2.2. Existing heuristics

Many algorithms are designed for USApHMP [18, 19, 20, 21, 22]. Such as: simulated annealing (SA) [23], tabu search (TS) [24] and Variable neighborhood search (VNS) [25, 56]. The VNS was used to solve several optimization problems [26] for example, mixed integer programming [27], scheduling problem [28].

If the variable neighborhood descent (VND) is used instead of a simple local search, and then the initial solution is improved by VNS, the general neighborhood variable search scheme (GVNS) is obtained, indicating that GVNS is a broader version of the basic VNS.

A real-world application of the GVNS is shown for one-commodity pickup –and- delivery traveling salesman problem [29]. This includes considering the feasibility of a possible traveling salesman's tour for the travel and designing the optimal travel tour. It can to solve instances with up to 1000 customers. Also, GVNS is provided by [30] proposed to address continuous optimization. In [31]

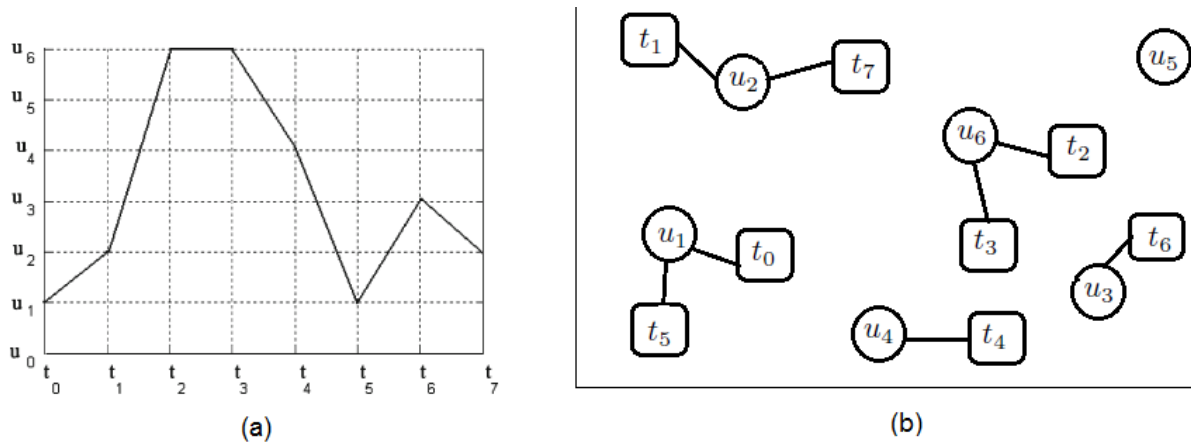


Figure 1: (a) Typical discretization NOCP with $n = 7$ and $m = 6$ and (b) considering NOCP as USApHMP.

sequential general variable neighborhood search (SGVNS) was studied for USApHMP and showed better than some algorithms.

Because of the diversity of the algorithms and the ability to solve useful problems and structural similarity with USApHMP and CSTR, the two-phase modified SGVNS denoted as MSGVNS method for solving CSTR is considered. We survey a different number of time nodes in two phases. The algorithm starts with a small number of time nodes in the phase1 and can reduce computational time by finding a better option for controllers.

3. MSGVNS algorithm

In this section, the components of two-phase MSGVNS algorithm of solving the USApHMP are described. This algorithm uses a standard sequential variable neighborhood descent (SVND). Three local neighborhood search are examined in the SVND.

3.1. Sequential general variable neighborhood search

Variable neighborhood descent (VND) is a deterministic variant of VNS that uses $l_{max} \geq 2$ neighborhood structures in the local search [32]. We used three local searches to increase the variety of solutions obtained in the following:

Neighborhood structures

A neighborhood structure is designed by introducing motion from one solution to another in local search. The final solution is provided when a local optimum cannot be improved using the neighborhood structure.

Note that two of the neighborhood structures, the first and the second, are the same as the *allocate* and *alternate*[31] and the same as $G_{reassign}$ and $G_{replace}$ neighborhoods [33]. However, these neighborhoods are applied in a different order and the third local search is the new one, the basic neighborhood structures for CSTR is as followed:

- The first local search method within VND, is as follow. This local change does not modify the selected controls. For all n time sections, we try to change its membership. This means that we select the t_i time node and try to replace the u_k assignments, so all other time nodes remain unchanged. When calculating new cost performance, we can calculate the cost difference between old and new assignments.

- In the second local search method, a u_k control is changed, and if the cost function decreases, we move to this neighborhood solution. In the first step, a control such as u_j that is not in u_0, \dots, u_p and a random control u_k from u_0, \dots, u_p is selected. From the current assignment set, we can modify all time nodes for u_k and then change its control to u_j . All controls from u_0, \dots, u_p are selected exactly once. Therefore, the change in cost performance is calculated for the new u_j .
- In the third local search, one u_j that is not in u_0, \dots, u_p and a random control u_k from u_0, \dots, u_p are selected. u_k is replaced with u_j and all time nodes are reassigned to the random control (including the new one). Thus all assignments are changed and the new cost function calculate. As mentioned above, the local search ends if there is no further progress in the third neighborhood.

The usual strategy for exploration of several neighborhoods within certain local search is sequential because the neighborhood structures are explored one by one which sequential VND (SVND) is found in Algorithm 1 [34, 26].

The pseudo-code for solving CSTR by SGVNS heuristic that using SVND in the local search step can be expressed as follows.

Algorithm 1: The phase 1 of SGVNS method

Input: Select k_{max} and it_{max} , find an initial solution

```

1  $k = 1$ 
2  $i = 1$ 
3 While  $i < it_{max}$  do
4   Generate a random assignment in  $k$ -th neighborhood
5    $j = 1$ 
6   While  $j < 4$  do
7     If  $j = 1$  then
8       Apply the first local search on current assignment
9     else If  $j = 2$  then
10      Apply the second local search on current assignment
11    else If  $j = 3$  then
12      Apply the third local search on current assignment
13     $j=j+1$ 
14    Update current assignment and  $j = 1$ 
15   $k=k+1$ 
16  if the current assignment is better than solution then
17    Update current solution and  $k = 1$ 
18  if  $k = k_{max} + 1$  then
19     $k = 1$ 
20   $i=i+1$ 

```

3.2. Modified SGVNS

Because a CSTR model may have various possible solutions, obtaining at least some of them rather requires a large set of initial conjectures across the domain. Applying possible physical values for system parameters, as in the case of CSTR can determine the existence of at least one feasible solution to the problem. Thus, we now give the two-phase solving strategy in Algorithm 2, MSGVNS, with a random initial solution constructed by (2.9) to gain feasible solutions for the search space in possible computational time. After visiting the initial solution, we use a method similar to [31, 29] to generate a new solution because on average it offers better results than some of the algorithms. Since the main aim in phase 1, is to find a hopeful solution in the search space with short computational times, a few numbers of partition time are used (see Algorithm 1). However, when a feasible

solution is reached, we restrict our search to the subspace of the obtained solution.

Next, to manage the quality of the solution for a CSTR model, we use phase 2 from a point reached in phase 1 and so increase the accuracy of this solution. So, after obtaining the feasible solution in phase 1, in phase 2, the values of the new domain boundary of the control of solution (i.e. b_{min} and b_{max}) are divided into n parts. Then the interval $[b_{min}, b_{max}]$ are divided to n number of partition and the solution with the modified control partition set is considered as the initial solution and Phase 1 restarts to find a better one in low computational times. Finally, with our new local search in MSGVNS, we find better results than the method proposed in [35, 36, 37, 38, 39] for CSTR.

Algorithm 2: The algorithm of the MSGVNS method

Input: Select Input r_{max} .

```

1  $r = 1$ 
2 While  $r < r_{max}$  do
3   phase 1: Perform SGVNS (Algorithm 1) with a random initial solution and new  $u_{min}$  and
      $u_{max}$ 
4   If the current solution is better than initial solution
5     Update current solution
6     construct initial solution for phase 2:
7        $u_{min} = b_{min}$  ;
8        $u_{max} = b_{max}$ ;
9    $r = r + 1$ 

```

The MSGVNS uses the three neighborhood structures that explained above (as stated in Algorithm 1).

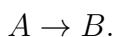
Importance of the new neighborhood structure: this paper introduces the new neighborhood structure that was the third local structure and it gives better results. Algorithm use the two parameters, i.e., $k_{max} = 30$, $it_{max} = 10$ and $r_{max} = 10$ for each problem instance. We showed the two-phase algorithm with a few amounts of k_{max} , and it_{max} can solve CSTR in less computational time. Table 1-3 show the following: other methods, the best solution, the computational time.

Remark. All metaheuristics are interesting because of their numerical behavior, and after a few iterations, they get good results. There is no particular theory of VNS convergence, nor is there any general assumption about the convergence of metaheuristic algorithms [40, 41]. Although in [42] a simple structure is organized for global convergence of VNS based on the concept of absorption probabilities .

4. CSTR examples

4.1. Constrained first-order CSTR

This dynamic optimization problem is an irreversible first-order CSTR chemical reaction that is first formulated by [43, 13]. An irreversible reaction, the single reactive material is shown as follows:



According to [13], (2.1) - (2.2) may be express into dimensionless form and, through a selection of a fit set of parameters, the equations describing the chemical reactor are:

$$\begin{aligned} \dot{x}_1 &= (-2 + u)(x_1 + 0.25) + (x_2 + 0.5) \exp\left(\frac{25x_1}{x_1 + 2}\right), \\ \dot{x}_2 &= 0.5 - x_2 - (x_2 + 0.5) \exp\left(\frac{25x_1}{x_1 + 2}\right). \end{aligned}$$

If the amount of coolant flow entering the reactor through the coil is changed, then the $u(t)$ control variable, which depends on the valve opening, also changes. There are two state variables $x_1(t)$ and $x_2(t)$ that express the deviation from the dimensionless steady-state temperature and concentration. The goal of CSTR is to determine a control function $u(t)$ that transfers the system from initial condition $(x_1(0), x_2(0)) = (0.09, 0.09)$ and interval time $[0, 0.78]$ that minimizes the following performance index:

$$g = \int_{t_0}^{t_f} (x_1^2 + x_2^2 + 0.1u^2)dt.$$

As was shown by [44], this system donates a local minimum $J = 0.24425$ and a minimum $J = 0.133094$ when Pontryagin's maximum principle is used. A simple approach, based on Pontryagin's maximum principle, was applied by [45] to obtain an initial guess for the solution, then the minimum value of $J = 0.1334$ was obtained.

This problem was solved by [11] applying eight stochastic global optimization methods, so the results received ranging between $J = 0.135$ and $J = 0.245$. The problem has been solved by the MSGVNS with $[0, 5]$ as the control interval. The best result for $n = 70, m = 30$ is $J^* = 0.0318$ that is better than other solution. We have also compared our result with other algorithms. It is clear that the

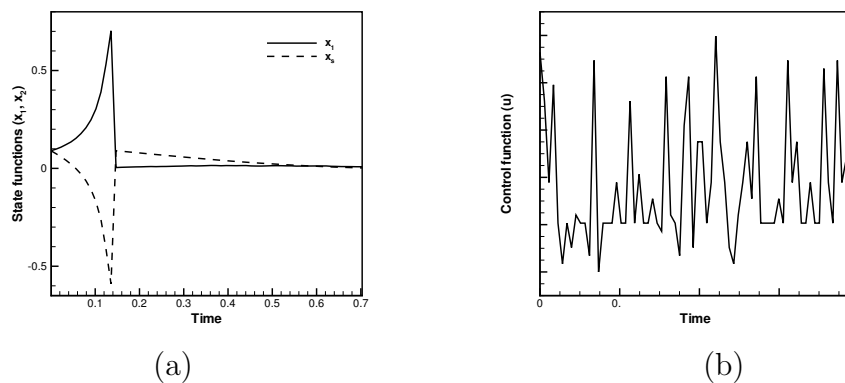


Figure 2: Figure of consecutive reaction batch reactor dynamic optimization problem: (a) The resulting optimal trajectories, (b) The resulting optimal control

performance index, J , for the MSGVNS methods are more accurate than IPSO ([46]), $J = 0.1355$ and LI $J = 0.1307$ ([38]) and WOA $J = 0.133724$ ([47]). Figure 2-(a) shows the control function for the optimal solution obtained by our method. The corresponding state trajectories were also given in Figure 2-(b). Compared with other methods, the MSGVNS has both faster convergence speed and better results although Figure 3 shows the convergence behavior of our method for 40 iterations.

4.2. Unconstrained two-state variable mathematical system.

Some researchers have studied the problem of consecutive reaction batch reactor dynamic optimization that the reaction $A \rightarrow B \rightarrow C$ occurs [49, 50]. In this model, it is necessary to find the

Table 1: Comparison of results for the nonlinear continuous stirred-tank reactor dynamic optimization problem

Algorithm	Computation time (s)	Final solution
Method of [38]	30.6	0.1307
Differential Evolution Algorithm [48]	NR	0.1358
The proposed method	300	0.0368

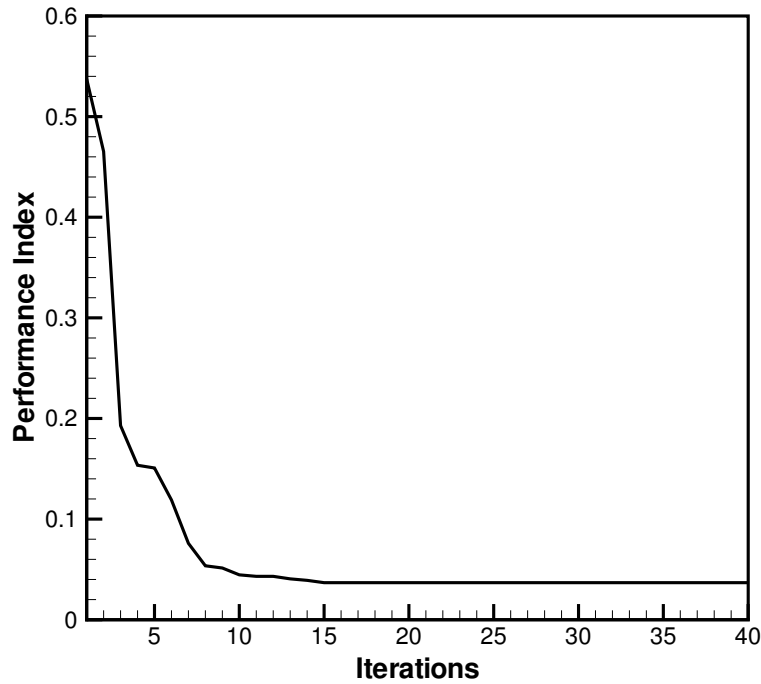


Figure 3: Convergence of the performance index for the consecutive reaction batch reactor dynamic optimization problem

optimal temperature profile that maximizes product performance of B temperature at the result of the process in the batch reactor. To maximize the cost performance, the feed rate u in $t \in [0, 1]$ is as follows:

$$J(u) = x_1(t_f).$$

The control and state functions are respectively input and the response of the following dynamical system:

$$\begin{aligned} \dot{x}_1 &= -620000e^{\left(\frac{-5000}{u}\right)} x_1 + 4000e^{\left(\frac{-2500}{u}\right)} x_2^2, \\ \dot{x}_2 &= -4000e^{\left(\frac{-2500}{u}\right)} x_2^2. \end{aligned}$$

The problem has two state constraints with initial condition, $[x_1, x_2]^T = [0, 1]^T$, where x_1 shows the concentration of B , x_2 represents the concentration of A ; u is the temperature in [298, 398].

The optimal value for HIGA [51] was obtained as 0.61046, which was more accurate than iterative ACO [50] and ACO [52]. The optimal value in [39] drives to solution 0.6107 with 102 iterations and the maximum solution obtained from the hybrid stochastic optimization method in [37] is 0.6128. The best obtained values by [38] for LI and SI are 0.61067 and 0.61078 respectively, which is better than HIGA. To compare the performance of MSGVNS to existing methods, the comparison results are given in Table 1. The maximum value by applying MSGVNS is $J^* = 0.7968$ was obtained very rapidly. The computation time with a discretization of $n = 9, m = 30$ subintervals, was 179 seconds.

In addition, we present our approach to the optimal control in Figure 4-(b) and the resulting state trajectories in Figure 4-(a). The result from the approach of [37] and [39] are 0.6107 and 0.6128 that

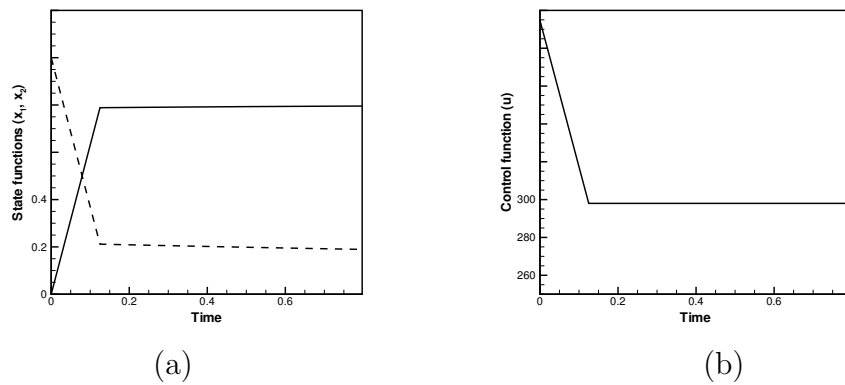


Figure 4: Figure of consecutive reaction batch reactor dynamic optimization problem: (a) The resulting optimal trajectories, (b) The resulting optimal control

is exceeded by our method to 0.7968 that shown in Table 2. Figure 5 shows the resulting performance index for iterations that the convergence occurs before the 15th iteration.

4.3. Photochemical CSTR

A challenging subject of higher dimensions involves a photochemical reaction in an isothermal CSTR that is used for optimal control problems in [13, 53] formulated by [54]. Four control variables of the CSTR is surveyed to determine for maximizing the economic benefit that has been studied by some researchers [55, 39]. Several chemical reactions simultaneously show the dynamics of the system. For maximizing the cost function, four control inputs $u_i, i = 1, \dots, 4$ are, respectively, the electrical energy input and the flow rate of three feed streams over $t \in [0, 0.2]$ is selected:

$$J(u) = x_1(t_f),$$

subject to:

$$\begin{aligned} \dot{x}_1 &= 5.8[(u_1 + u_2 + u_3)x_2 - u_1] - 3.7u_2 - 4.1u_3 \\ &\quad + (u_1 + u_2 + u_3)(23x_5 + 11x_6 + 28x_7 + 35x_8) - 5u_4^2 - 0.099, \\ \dot{x}_2 &= u_1 - (u_1 + u_2 + u_3)x_2 - 17.6x_2x_3 - 23x_2x_7u_4, \\ \dot{x}_3 &= u_2 - (u_1 + u_2 + u_3)x_3 - 17.6x_2x_3 - 146x_3x_4, \\ \dot{x}_4 &= u_3 - (u_1 + u_2 + u_3)x_4 - 73x_3x_4, \\ \dot{x}_5 &= -(u_1 + u_2 + u_3)x_5 + 35.2x_2x_3 - 51.3x_5x_6, \\ \dot{x}_6 &= -(u_1 + u_2 + u_3)x_6 + 219x_3x_4 - 51.3x_5x_6, \\ \dot{x}_7 &= -(u_1 + u_2 + u_3)x_7 + 102.6x_5x_6 - 23x_2x_7u_4, \\ \dot{x}_8 &= -(u_1 + u_2 + u_3)x_8 + 46x_2x_7u_4, \end{aligned}$$

Table 2: Comparison of results for the unconstrained two-state variable system

Algorithm	Computation time (s)	Final solution
Method of [39]	653	0.6107
Hybrid stochastic optimization method [37]	385	0.6128
The proposed method	179	0.7968

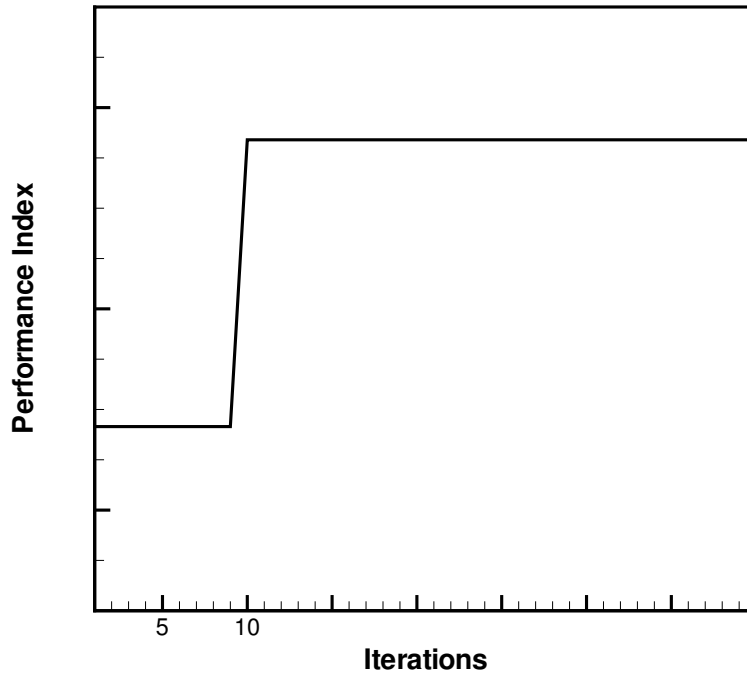


Figure 5: Convergence of the performance index for the consecutive reaction batch reactor dynamic optimization problem

and the control input constraint

$$\begin{aligned}
 0 &\leq u_1 \leq 20, \\
 0 &\leq u_2 \leq 20, \\
 0 &\leq u_3 \leq 6, \\
 0 &\leq u_4 \leq 4,
 \end{aligned}$$

with the initial condition

$$x(0) = [0.0000, 0.1883, 0.2507, 0.0467, 0.0899, 0.1804, 0.1394, 0.1046]^T .$$

the maximum value for the performance index in [36] by using piecewise constant control with $n = 11$ time stages of equal length was 21.75722. The problem has been solved by the proposed method with $n = 9$ and $p_1 = p_2 = p_3 = p_4 = 10$ (number partition of u_1, u_2, u_3, u_4). The optimal control was shown in Figure 7-(a) and corresponding trajectories were given in Figure 6. To compare the performance of our method to existing methods, the results of [37, 39] were shown in Table 3. The comparison of results are given by figures and Table 3 explains that MSGVNS takes 330s to give the satisfactory solution 22.24, but the method of [39] takes 2493s to arrive the local optimal 21.8241 and [37] takes 1346s for local optimal solution 21.85. In addition, Table 3 shows that the results of the implementation of other methods are exceeded by our method to 22.24, indicating 2% improvement in the objective function. Figure 7-(b) shows the convergence of MSGVNS for 80 iterations.

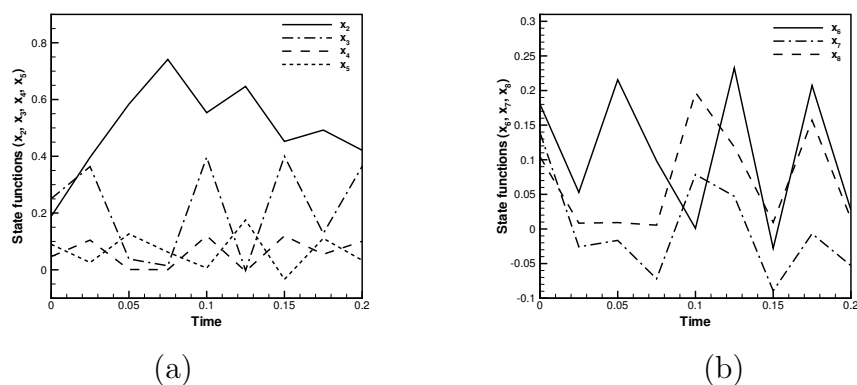


Figure 6: Figure of consecutive reaction batch reactor dynamic optimization problem: (a),(b) The resulting optimal trajectories

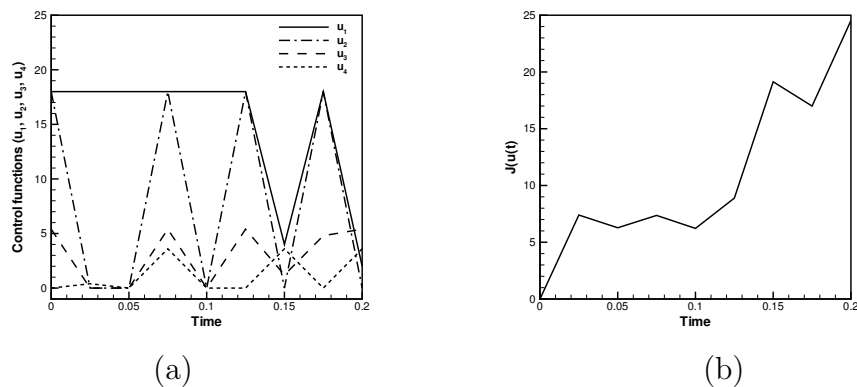


Figure 7: Figure of consecutive reaction batch reactor dynamic optimization problem: (a) The resulting optimal controls, (b) optimal performance index

5. Conclusion

The paper considers the chemical process system's optimal control problem. To solve the CSTR problem, a modified metaheuristic is considered. The similarity structure USApHMP with CSTR, persuade us to make modifications to one of the successful methods of solving the USApHMP and with this in mind that the cost structure shown in Figure 1., the two-phase MSGVNS algorithm was presented. The correctness of this view may be seen in the numerical results presented in Section 4. Our results match all previously known optimal solutions and best-known solutions for CSTRs and significantly improve best-known objective values for CSTRs in a few computing time. In general, the cost function of our approach is dependant on the value of n, m . Although, we find optimal solutions in fewer n, m than other methods. Based on the above experimental results, we can infer that MSGVNS is effective and robust in terms of both solution quality and convergence speed. It

Table 3: Comparison of results for the nonlinear continuous stirred-tank reactor dynamic optimization problem

Algorithm	Computation time (s)	Final solution
Method of [39]	2493	21.8241
Hybrid stochastic optimization method [37]	1346	21.8503
The proposed method	330	22.24

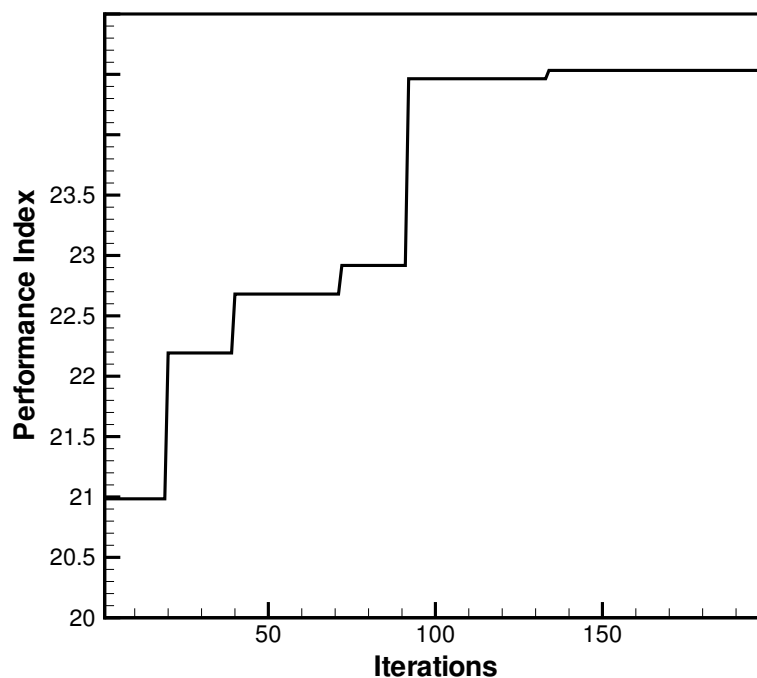


Figure 8: Convergence of the performance index for the consecutive reaction batch reactor dynamic optimization problem

seems that with the approach presented in this paper, in the next research, it is possible to reduce the shortcomings that metaheuristic methods have for finding approximate solutions in different types of chemical process. Also, with this type of view of the problem, it is easy to speed up the process of obtaining the approximate solutions by some schemes such as parallelization.

References

- [1] SA. Ravichandran, JJ. Krist, D. Edwards, S. Delagah and J. Pellegrino, *Measuring sparingly-soluble, aqueous salt crystallization kinetics using CSTRs-in-series: Methodology development and CaCO₃ studies*, Sep. Purif. Technol. 211 (2019) 408–420.
- [2] A. Regalado-Méndez, RR. Romero, RN. Rangel and S. Skogestad, *Biodiesel production in stirred tank chemical reactors: A numerical simulation*, In *New Trends in Networking, Computing, E-learning, Systems Sciences, and Engineering*, pp. 109–116, Springer, Cham, 2015.
- [3] Z. Cao, Q. Wu, H. Zhou, P. Chen and F. You, *Dynamic modeling, systematic analysis, and operation optimization for shell entrained-flow heavy residue gasifier*, (2020) Energy, 117220.
- [4] TM. Braden, MD. Johnson, ME. Kopach, J. McClary Groh, RD. Spencer, J. Lewis and J.J. Adler, *Development of a commercial flow Barbier process for a pharmaceutical intermediate*, Org. Process. Res. Dev. 21(3) (2017) 317–326.
- [5] D. Gola, P. Chawla, A. Malik and SZ. Ahammad, *Development and performance evaluation of native microbial consortium for multi metal removal in lab scale aerobic and anaerobic bioreactor*, Environ. Technol. Innov. (2020) 100714.
- [6] I. Malinen, J. Kangas, J. Ahola and J. Tanskanen, *A new homotopy-based strategy for the robust determination of all the feasible solutions for CSTR systems*, Period. Polytech. Chem. 60(1) (2016) 8–23.
- [7] A. Uppal, WH. Ray and AB. Poore, *On the dynamic behavior of continuous stirred tank reactors*, Chem. Eng. Sci. 29(4) (1974) 967–985.
- [8] K. Pathak, A. Markana, N. Parikh, *Optimal control of CSTR*, Nirma Univ. J. Eng. Technol. 1(2) (2010) 56–60.

- [9] ZS. Abo-Hammour, AG. Asafteh, AM. Al-Smadi, and OM. Alsmadi, *A novel continuous genetic algorithm for the solution of optimal control problems*, Optim. Contr. Appl. Met. 32(4) (2011) 414–432.
- [10] A. Uppal, WH. Ray and AB. Poore, *The classification of the dynamic behavior of continuous stirred tank reactors—influence of reactor residence time*, Chem. Eng. Sci. 31(3) (1976) 205–214.
- [11] MM Ali, C. Storey and A. Törn, *Application of stochastic global optimization algorithms to practical problems*, J. Optimiz. Theory. App. 95(3) (1997) 545–563.
- [12] CA. Floudas, PM. Pardalos, CS. Adjimann, WR. Esposito, ZH. Gumus, ST. Harding and CA. Schweiger, *Handbook of test problems in local and global optimization*, 1999, 67.
- [13] L. Lapidus, R. Luus, *Optimal control of engineering processes* (1967) (No. 629.8 L3).
- [14] M. Salimi, AH. Borzabadi, HH. Mehne and A. Heydari, *The hub location's method for solving optimal control problems*, Evol. Intel. (2020) 1–20
- [15] EZ. Serper and SA. Alumur, *The design of capacitated intermodal hub networks with different vehicle types*, Transport. Res. Part B: Methodological, 86 (2016) 51–65.
- [16] S. Alumur and BY. Kara, *Network hub location problems: The state of the art*, Eur. J. Oper. Res. 190(1) (2008) 1–21.
- [17] RZ. Farahani, M. Hekmatfar, AB. Arabani, E. Nikbakhsh, *Hub location problems: A review of models, classification, solution techniques, and applications*, Comput. Ind. Eng. 64(4) (2013) 1096–1109.
- [18] JF. Campbell, *Hub location and the p-hub median problem* Oper. Res. 44(6) (1996) 923–935.
- [19] J. Kratica, Z. Stanimirović, D. Tošić and V. Filipović, *Two genetic algorithms for solving the uncapacitated single allocation p-hub median problem*, Eur. J. Oper. Res. 182(1) (2007) 15–28.
- [20] Z. Stanimirovic, *A genetic algorithm approach for the capacitated single allocation p-hub median problem*, Comput. Inform. 29 (1) (2010) 117–132.
- [21] J. Rieck, C. Ehrenberg and J. Zimmermann, *Many-to-many location-routing with inter-hub transport and multi-commodity pickup-and-delivery*, Eur. J. Oper. Res. 236(3) (2014) 863–878.
- [22] H. Karimi and M. Setak, *Proprietor and customer costs in the incomplete hub location-routing network topology*, Appl. Math. Model. 38(3) (2014) 1011–1023.
- [23] AT. Ernst and M. Krishnamoorthy, *Efficient algorithms for the uncapacitated single allocation p-hub median problem*, Location science, 4(3) (1996) 139–154.
- [24] D. Skorin-Kapov and J. Skorin-Kapov, *On tabu search for the location of interacting hub facilities*, Eur. J. Oper. Res. 73(3) (1994) 502–509.
- [25] MP. Pérez, FA. Rodríguez and JMM Vega, *On the use of path relinking for the ρ -hub median problem*, In *European Conference on Evolutionary Computation in Combinatorial Optimization*, pp.155–164, 2004.
- [26] P. Hansen, N. Mladenović and JAM. Pérez, *Variable neighbourhood search: methods and applications*, 4OR, 6(4) (2008) 319–360.
- [27] P. Hansen, N. Mladenović and D. Urošević, *Variable neighborhood search and local branching*, Comput. Oper. Res. 33(10) (2006) 3034–3045.
- [28] WE. Costa, MC. Goldberg and EG. Goldberg, *New VNS heuristic for total flowtime flowshop scheduling problem*, Expert. Syst. Appl. 39(9) (2012) 8149–8161.
- [29] N. Mladenović, D. Urošević and A. Ilić, *A general variable neighborhood search for the one-commodity pickup-and-delivery travelling salesman problem*, Eur. J. Oper. Res. 220(1) (2012) 270–285.
- [30] N. Mladenović, M. Dražić, V. Kovačević-Vujčić and M. Čangalović, *General variable neighborhood search for the continuous optimization*, Eur. J. Oper. Res. 191(3), (2008), 753–770.
- [31] A. Ilić, D. Urošević, J. Brimberg and N. Mladenović, *A general variable neighborhood search for solving the uncapacitated single allocation p-hub median problem*, Eur. J. Oper. Res. 206(2) (2010) 289–300.
- [32] N. Mladenović and P. Hansen, *Variable neighborhood search*, Comput. Oper. Res. 24(11) (1997) 1097–1100.
- [33] S. Wolf and P. Merz, *Evolutionary local search for the super-peer selection problem and the p-hub median problem*, In *International Workshop on Hybrid Metaheuristics*, pp.1–15, Springer, Berlin, Heidelberg, 2007.
- [34] P. Hansen and N. Mladenović, *Developments of variable neighborhood search*, In *Essays and surveys in metaheuristics*, pp.415–439, Springer, Boston, MA., 2002.
- [35] S. Nezhadhossein, A. Heydari and R. Ghanbari, *A modified hybrid genetic algorithm for solving nonlinear optimal control problems*, Math. Probl. Eng. (2015), 1–21.
- [36] R. Luus, *Iterative Dynamic Programming*, CRC Press, 2000.
- [37] X. Wu, B. Lei, K. Zhang and M. Cheng, *Hybrid stochastic optimization method for optimal control problems of chemical processes*, Chem. Eng. Res. Des. 126 (2017) 297–310.
- [38] S. Nezhadhossein, A. Heydari and R. Ghanbari, *Integrating Differential Evolution Algorithm with Modified Hybrid GA for Solving Nonlinear Optimal Control Problems*, Iran. J. Math. Sci. Inf. 12(1) (2017) 47–67.

- [39] E. Lazutkin, A. Geletu, S. Hopfgarten, and P. Li, *An analytical hessian and parallel-computing approach for efficient dynamic optimization based on control-variable correlation analysis*, Ind. Eng. Chem. Res. 54(48) (2015) 12086–12095.
- [40] AM. Johnson and SH. Jacobson, *On the convergence of generalized hill climbing algorithms*, Discrete. Appl. Math. 119(1-2) (2002) 37–57.
- [41] H. Muhlenbein and J. Zimmermann, *Size of neighborhood more important than temperature for stochastic local search*, In *Proceedings of the 2000 Congress on Evolutionary Computation*, (Cat. No. 00TH8512), 2, pp.1017–1024, IEEE, 2000.
- [42] J. Brimberg, P. Hansen and N. Mladenovic, *Attraction probabilities in variable neighborhood search*, 4OR 8(2) (2010) 181–194.
- [43] R. Aris and NR. Amundson, *An analysis of chemical reactor stability and control—III: The principles of programming reactor calculations, Some extensions*, Chem. Eng. Sci. 7(3) (1958) 148–155.
- [44] R. Luus and DE. Cormack, *Multiplicity of solutions resulting from the use of variational methods in optimal control problems*, Can. J. Chem. Eng. 50(2) (1972) 309–311.
- [45] L. Bayón, JM. Grau, M.M. Ruiz and PM. Suárez, *Initial guess of the solution of dynamic optimization of chemical processes*, J. Math. Chem. 48(1) (2010) 28–37.
- [46] H. Modares and MBN. Sistani, *Solving nonlinear optimal control problems using a hybrid IPSO–SQP algorithm*, Eng. Appl. Artif. Intel. 24(3) (2011) 476–484.
- [47] HH. Mehne and S. Mirjalili, *A parallel numerical method for solving optimal control problems based on whale optimization algorithm*, Knowl-Based. Syst. 151 (2018) 114–123.
- [48] IL. Cruz, LG. Van Willigenburg and G. Van Straten, *Efficient differential evolution algorithms for multimodal optimal control problems*, Appl. Soft. Comput. 3(2) (2003) 97–122.
- [49] SA. Dadebo and KB. McAuley *Dynamic optimization of constrained chemical engineering problems using dynamic programming*, Comput. Chem. Eng. 19(5) (1995) 513–525.
- [50] B. Zhang, D. Chen and W. Zhao, *Iterative ant-colony algorithm and its application to dynamic optimization of chemical process*, Comput. Chem. Eng. 29(10) (2005) 2078–2086.
- [51] S. Fan, D. Wenli, Q. Rongbin, Q. Feng and W. ZHONG, *A hybrid improved genetic algorithm and its application in dynamic optimization problems of chemical processes*, Chinese. J. Chem. Eng. 21(2) (2013) 144–154.
- [52] J. Rajesh, K. Gupta, HS. Kusumakar, VK. Jayaraman and BD. Kulkarni, *Dynamic optimization of chemical processes using ant colony framework*, Comput. Chem. 25(6) (2001) 583–595.
- [53] SN. Rao and R. Luus, *Evaluation and improvement of control vector iteration procedures for optimal control*, Can. J. Chem. Eng. 50(6) (1972) 777–784.
- [54] TB. Jensen, *Dynamic control of large dimension nonlinear chemical processes*, Doctoral dissertation, Princeton University, (1965).
- [55] X. Chen, W. Du, R. Qi, F. Qian and H. Tianfield, *Hybrid gradient particle swarm optimization for dynamic optimization problems of chemical processes*, Asia. Pac. J. Chem. Eng. 8(5) (2013) 708–720.
- [56] MP. Pérez, FA. Rodríguez and JM. Moreno-Vega, *A hybrid VNS–path relinking for the p-hub median problem*, IMA. J. Manag. Math. 18(2) (2007) 157–171.