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Optimization of flexible square cascade for high separation of stable isotopes using enhanced PSO algorithm

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ABSTRACT

The optimal parameters of a flexible square cascade for the separation of multicomponent isotopes have been calculated in this paper. In this regard, a new code called "MCSQCA-PSO" has been developed, which uses the particle swarm algorithm with mutation operator to find the optimal solution. Maximizing the amount of product recovery in a square cascade with the certain number of centrifuges machines and considering the concentration of the desired isotope in specific values, as well as increasing the D function as an objective function have been evaluated and studied. Cascade feed flow rate, machine feed flow rate, cascade cut, feed entrance point, and stages cut have been defined as optimization variables in the code. Optimization calculations are performed as an example for separation of Te-123, which has the most challenging separation between the eight stable isotopes of tellurium. In this paper, all possible arrangements of a square cascade assuming 200 centrifuges for two different separation factors have been investigated, and the enrichment of Te-123 has been increased from 0.89 % in natural feed to 65 %. The results show that the recovery coefficient increases nonlinearly with increasing the number of stages from 10 to 100, so that it is not significantly different for cascades in 40, 50, and 100 stages. In contrast, the amount of product in the cascade with 50 stages is the highest in comparison with the other cascades. Finally, the recovery coefficients of Te-123 in the cascade with 50 stages for two different separation factors have obtained 99.46 % and 92.38 %, respectively. The amount of product after two steps of separation and assuming one year of operation have been obtained 4.6 kg and 4.1, respectively. Furthermore, the ability of MCSQCA-PSO is evaluated with other optimization algorithms. Suitable alignment of the results indicates that the use of the PSO for this problem guarantees the calculation of the optimal parameters.

1. Introduction

In recent years, the demand for the production of stable isotopes with high concentrations has increased. The stable isotopes are used in medicine as precursors for radioisotopes, for magnetic imaging, in electronic, and physics researches, etc. (Mol and Rakhorst, 2003; Sulaberidze and Borisevich, 2001).

Various methods have also been introduced for designing the cascades in multicomponent isotopes separation such as the R-cascade, the Q-cascade, and the quasi-ideal cascade, among which the use of a square cascade is practical (Azizov et al., 2020a, b; Sulaberidze and Borisevich, 2001). Due to the return flows in the first and last stages, the square cascades can be used in low feeds, and also by different cuts. This leads to high flexibility in operation, and therefore, square cascades are suitable for the separation of stable isotopes in a wide range. In the flexible cascade the feed rate and its location changed alternately, and the desired component separated step by step.

Because of the flexible square cascade structure, it is necessary to be calculated the optimal parameters that can be changed at each step (including the cascade feed flow rate, feed location, feed flow rate of gas centrifuges, the cut of stages, and the cascade cut) and for each process material, distinctly. Therefore, finding the cascade with the best performance is always of interest to separate the multicomponent mixtures. In the multicomponent mixture separation, it is best to develop particular methods that take into account the given criteria for optimization and to investigate new codes with regard to the importance of the design an optimum cascade. The cascade design is a constrained multi-objective optimization. By means of the optimization techniques, it is possible to create an optimum cascade with adequate performance based on the specific features of the gas centrifuges in use (Palkin, 2013;

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Palkin and Maslyukov, 2014; Song et al., 2010; Mansourzadeh et al., 2019).

In 2000, Palkin and Rozenbaum introduced the necessary relations which make it possible to implement the numerical-analytical method for determining the optimal parameters of a cascade of centrifuges with optimal separation power and strictly fixed external parameters of cascades. In 2002, Palkin et al. used Hooke–Jeeves method for optimization of a square cascade parameters with a specified concentration of a desired component in the outgoing flows. In 2018, Sulaberidze et al. optimized tapered cascades with variable overall separation. The optimization criterion was the minimum total separation capacity in the cascade. Safdari et al., in 2017, directly applied the results of the purely axial flow model in a single gas centrifuge to achieve the separation factor in relation to θ and f and optimize the taper cascade using PSO algorithm. Mansourzadeh et al., in 2018, optimized the taper cascade and compared the results with the square cascade for the separation of xenon isotopes. In 2019, the intermediate total flow rate considering desired isotope concentration has investigated as the objective function for optimizing a taper cascade using HS algorithm, by Mansourzadeh et al.

In 2020, Azizov et al. optimized a single square cascade with a specified configuration in order to avoid searching the initial approximation for the concentration of the components in the in outgoing flows. Optimizing a system of three square cascade was done by Azizov et al., for the constant separation factor that the number of the stages in each step has been changed, and the enrichment of target isotope was determined using the model cascades in each step (Azizov et al., 2020b). In 2020, Imani et al. optimized a non-conventional square cascade with the PSO algorithm to reach the maximum product. Ezazi et al. used the ABC algorithm to optimize a taper cascade by applying the conditions of the matched-X cascade. In 2020, Palkin et al. optimized a cascade with two additional flows and concluded that bee swarm optimization has an advantage over the Hook-Jeeves method. In 2020, Palkin introduced a method for optimizing a cascade with two additional product streams, in which two components of intermediate-mass are concentrated simultaneously. The solution of the optimization problem was based on a variation of the flow partial cuts of the cascade stages with large separation factors. Minimum total feed stream of the stages with a specified concentration of the isotopes was used as the optimization criterion. In 2021, Dadashzadeh et al. utilized the GWO algorithm for minimizing the number of gas centrifuges in a taper cascade.

On the other hand, in the stable isotope separation, it is always necessary to have a high concentration of the desired isotope. That's because these isotopes would be used in medical applications for radioisotope production and it is important to be pure. For example, in the ^{124}Xe case which has a very small (equal to ~0.09 %) natural concentration, the separation process is conducted in several steps to be enriched more than 99.99 %. This isotope with high concentration use for production of radioisotope ^{123}I which has a wide range of medical applications. In the stable isotope separation, especially for middle isotopes separation, enriching to a high concentration is not possible with a single cascade and it must be done several times to reach a desired concentration. Moreover, the cost of the natural feed material is high for some elements and it is better to have a high recovery of the target isotope.

In this research, attempts have been made to overcome these two major challenges, and it leads us to use optimization algorithms for cascade design. Unlike other research works in this area that are mentioned before, in this paper, the main focus is on the optimization of multiple square cascades simultaneously, considering a new format of the objective function which has the ability to maximize the desired isotope recovery. Moreover, the concentration of the desired isotope among steps is unknown and the introduced optimization method of all steps simultaneously removes the need of providing extra information. These inter-step concentrations are calculated and optimized automatically based on the objective function.

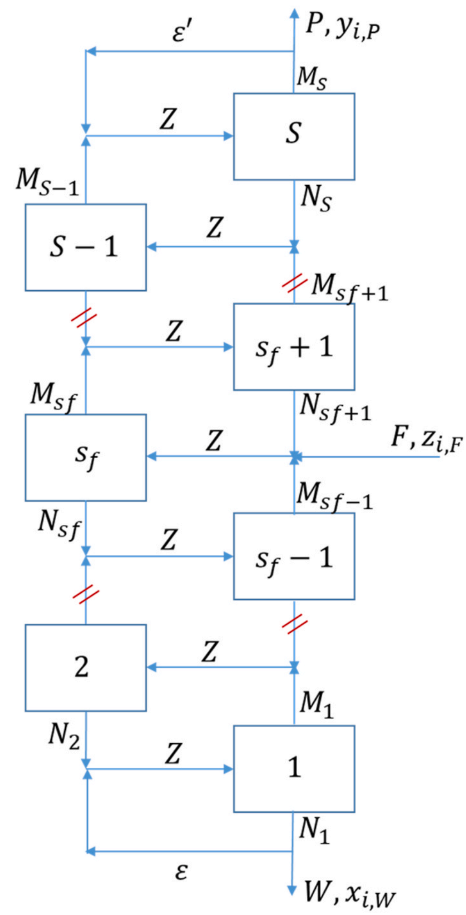

Fig. 1. A view of a common square cascade.

In this regard, an efficient code titled "MCSQCA-PSO" has been developed that can optimize the parameters of a flexible square cascade to separate all stable multicomponent isotopes. Maximizing the parameter D and increasing the product recovery coefficient considering the specific target isotope is selected as the objective function. In this code, after comparing different optimization algorithms and with a look at the reported application of this algorithm on taper cascade optimization, the PSO algorithm has been chosen for optimization. The PSO algorithm has been successfully employed for optimizing a wide range of engineering issues (Eberhart and Kennedy, 1995; Gao et al., 2019; Harrison et al., 2018; Khoshahval et al., 2010). In order to confirm the validity of proposed code, the results of the MCSQCA-PSO, are compared with the values reported by Azizov et al. (2020a), as well as some other optimization algorithms. To express the capability and computational efficiency of the proposed code, calculations are performed for separation of the third isotope of tellurium, in which the enrichment of Te-123 has been increased from 0.89 % in the natural feed to 65 %. Using this method, it is possible to increase the enrichment of each isotope at any concentration.

2. Theory

In this section, the governing equations of the square cascade to separate multicomponent isotopes have been expressed, and at the end, the D function is introduced.

The number of centrifuges in each stage and the feed flow rate in to them is constant in the square cascades (see Equation (1)). A view of the square cascade is given in Fig. 1 (Manson et al., 1981), where the feed stream at a rate of F enters in to the stage of s_f with composition $z_{i,F}$. The cascade delivers the product (P) and waste streams (W) with compositions $y_{i,p}$, $x_{i,w}$, respectively. In the following equations, the number of isotopes in the feed stream is N_c, and the total number of cascade stages is S. The feed flow rate to stage s is Z_s and the inter stage up and down flow rates are denoted by M_s and N_s.

2.1. Governing equations

The square cascades equations are explained in two separate sections. These include the flow and concentration survival equations.

2.1.1. Flow equations

In a symmetric cascade the flow rate of pipes can be obtained by the following equations for the cascade with certain cut stages, external feed and feed point. Equations (2)–(5) show the material balance the flow at intersections. Using the definition of cut and flow survival in stages, relations (6) and (7) will be obtained. In these relationships, θ_s refers to the stages cut. Also, the parameters ε and ε′ represent the return flows in the first and last stages of the square cascade, respectively (Mansourzadeh et al., 2018).

$$Z_1 = Z_2 = \dots = Z_S = Z \tag{1}$$

$$Z = M_{s-1} + N_{s+1} \quad , s \neq s_f \tag{2}$$

$$Z = M_{s-1} + N_{s+1} + F \ , s = s_f \tag{3}$$

$$Z = M_{S-1} + \varepsilon' \quad , s = S \tag{4}$$

$$Z = N_2 + \varepsilon \quad , s = 1 \tag{5}$$

$$M_s = Z\theta_s \tag{6}$$

$$N_s = Z(1 - \theta_s) \tag{7}$$

From Equations (2), (3) and (6), we have:

$$\theta_s = \theta_{s+2} \quad , s \neq s_f \tag{8}$$

$$\theta_{s-1} = \theta_{s+1} - \frac{F}{Z} \ , s = s_f \tag{9}$$

According to Equation (8), the cut of each stage will be equal to the cut in the next two stages. Moreover, the cut of stages before and after feed entrance follows the relation (9). Therefore, in a square cascade, the maximum cut values will be 3, and in general, the following conditions could be obtained (see Table 1):

From equations (1)–(7), the flow rates M_s, N_s, and the parameters ε and ε′ are unknown. Hence, in a square cascade with the S stages, there are 2S + 2 unknown. The sum of independent equations, which include the flow equations at the stages and intersections, is 2S. Therefore, in order to solve the equations, 2 parameters must be determined. One of the essential operational parameters in a square cascade is the cut of stages. Therefore, according to the Equations (10)–(12), having two cuts of the first and second stages, the flow rates could be obtained. From the survival of the flow in the last stage, Equation (13) is established. So, it can be used the cascade cut as an input parameter instead of the second stage cut.

$$W = Z(1 - \theta_1 - \theta_2) \tag{13}$$

2.1.2. Concentration equations

Equation (14) relates to the mass balance for the component ith in the stage nth:

$$Zz_{i,s} = M_s y_{i,s} + N_s x_{i,s} \tag{14}$$

Equations (15)–(18) show the relations of mass balance at the flow mixing points.

$$Zz_{i,s} = M_{s-1}y_{i,s-1} + N_{s+1}x_{i,s+1} + Fz_{i,F}, s = s_f \tag{15}$$

$$Zz_{i,s} = M_{s-1}y_{i,s-1} + N_{s+1}x_{i,s+1} \quad , s \neq s_f \tag{16}$$

$$Zz_{i,s} - M_{s-1}y_{i,s-1} - \varepsilon' y_{i,P} = 0, \quad s = S \tag{17}$$

$$Zz_{i,s} - N_{s+1}x_{i,s+1} - \varepsilon x_{i,w} = 0, \quad s = 1 \tag{18}$$

The relation of the separation factor is in the form of Equation (19), and the concentrations should satisfy the constraints in Equation (20).

$$\alpha_{ij,s} = \frac{(y_{i,s}/y_{j,s})}{(x_{i,s}/x_{j,s})} = \alpha_{0,s}^{(M_j - M_i)} \ , (i = j-1, \ j = 2, \dots, N_c) \tag{19}$$

$$\sum_{i=1}^{N_c} z_{i,s} = \sum_{i=1}^{N_c} y_{i,s} = \sum_{i=1}^{N_c} x_{i,s} = 1 \tag{20}$$

In this part of the equations, the values of isotopes concentrations in all stages could be calculated having the flow rates in all stages.

2.2. D function

To separate the middle components, the mixture of isotopes should be divided into two groups so that in one group, the desired middle component becomes an end component. For evaluating to what extent the two groups are separated from each other, function D was proposed by Zeng and Ying (2002). The mathematical expression of the D function is as follow:

$$D = \frac{P}{F}\sum_{i=1}^{k} y_{i,P} + \frac{W}{F}\sum_{i=k+1}^{N_c} x_{i,W} \tag{21}$$

When the two groups of light and heavy are completely separated from each other, the value of D becomes one, and we will have:

Table 1
Relation the cut of stages in a square cascade.

$s_f = odd$	$\theta_1 = \theta_3 = \theta_5 = \theta_{sf} = \theta_{sf+2}\dots$ $\theta_2 = \theta_4 = \dots = \theta_{sf-1} = \theta_{sf+1} - \frac{F}{Z} = \theta_{sf+3} - \frac{F}{Z}\dots$	**(10)**
$s_f = even$	$\theta_1 = \theta_3 = \dots = \theta_{sf-1} = \theta_{sf+1} - \frac{F}{Z} = \theta_{sf+3} - \frac{F}{Z}\dots$ $\theta_2 = \theta_4 = \theta_6 = \theta_{sf} = \theta_{sf+2}\dots$	(11)
$s_f = 1$ $s_f \neq 1$	$1 < \theta_1 + \theta_2 < 1 + \frac{F}{Z}$ $1 - \frac{F}{Z} < \theta_1 + \theta_2 < 1$	(12)

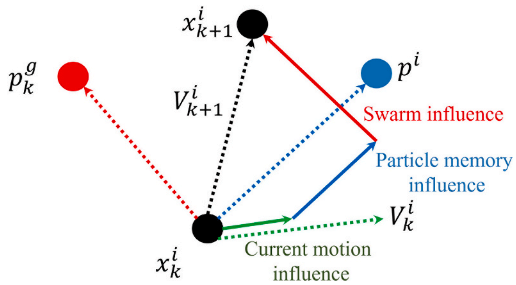

Fig. 2. Motion pattern in the particle swarm optimization algorithm.

$$\sum_{i=1}^{k} y_{i,P} = 1.0\ ,\ \sum_{i=k+1}^{N_c} x_{i,W} = 1.0 \tag{22}$$

3. Optimization

Particle swarm optimization is proposed in this paper to obtain the optimum parameters in a square cascade for multicomponent isotope separation. PSO has several advantages and can be used to solve nonlinear, nondifferentiable, and multipeak optimization problems, particularly in science and engineering fields (Eberhart and Shi, 2001; Harrison et al., 2018). This algorithm, has been successfully applied to a wide variety of optimization problems such as vehicle engineering, in-core fuel management, electric power systems, power economic dispatch, and footstep optimization for humanoid robots (Alrashidi and El-Hawary, 2009; Gao et al., 2019; Khoshahval et al., 2010; Lee and Kim, 2013; Park et al., 2005). Due to the capability of this algorithm in the taper cascade optimization (Safdari et al., 2017), PSO has also been used to optimize the square cascade parameters.

This section provides a brief description of PSO algorithm, the mutation operator used in it, and the new objective function used in this paper.

3.1. Particle swarm optimization algorithm

Like other dynamic techniques, the search algorithm is based on an initial population, and it starts with a population of random solutions to a problem called a particle (Eberhart and Shi, 2001; Kennedy and Eberhart, 1995). The algorithm begins by selecting a population of particles in the search space assigned to each particle location, velocity, and fitness value in the objective function. All particles know their best location, the best location of the group particles, and the value of the objective function. The particle behavior in this algorithm can be formulated according to Fig. 2 as follows (Eberhart and Kennedy, 1995; Kennedy and Eberhart, 1995):

a) Previous particle position, b) Particle distance to its best personal experience, c) Particle distance to the best experience of the whole population.

The mathematical expression of the above motion is in the form of the following relations:

$$v_i(t) = w \times v_i(t-1) + c_1 \times rand_1 \times \left(p_{i,best} - x_i(t-1)\right) + c_2 \times rand_2 \times \left(p_{g,best} - x_i(t-1)\right) \tag{23}$$

The parameters used in relation (23) are:

$v_i(t)$: The velocity of a particle in each iteration;

x_i: Particle location at each iteraion;

$c_1,\ c_2$:Acceleration constants, commonly referres to individual and collective learning coefficient and set to 2;

$rand_1,\ rand_2$: Random numbers between zero and one that changed at each itration;

w: Inertia weigh coefficient that modified in each iteration by $w = w \times w\_RF$; and set to 1;

w_RF: Inertia weight reduction factor that set to 0.99;

t: Current optimization stage number.

The above two commands are the same rules of self-organization in the particle swarm optimization algorithm, and all particles are required to implement it. For each new particle position, the best particle record (i, Best) and the best population record (Global Best) must be updated. In general, the following steps can be stated for the particle swarm optimization algorithm (Gao et al., 2019):

1 Set parameters w, w_RF, c_1 , and c_2
2 Creating an initial population and evaluating them;
3 Determining the best personal memory and the best collective memory;
4 Updating the speed and position and evaluating new answers;
5 If the stop conditions are not met, go to step 2, and otherwise;
6 The end.

3.2. Mutation operator

As many meta heuristics present problems of convergence to local optimal, the mutation operator is used to improve convergence of the PSO algorithm. In this algorithm, the mutation operates on a new population vector derived from the PSO algorithm. Mutation will help the population when it is trapped, so the population jumps to another position which may be away from the local optimum (Equation (24)). Initially, this operator generates a mutant population using Equation (25) with mu mutation. In other word, the number of parameters in the optimization vector that are mutated in each step is specified using Equation (25). mu is a random number with a normal distribution in the range 0–1. In this study, the value of mu is considered to be 0.1. For example, when the number of populations is considered to be equal to 50 in each itration, 0.1 of them use this operator. In the second step, the mutation operator selects the best population among the current optimal population obtained using the PSO algorithm (X_i). If the mutant population is better than X_i, X_i is replaced by X_{new}; Otherwise, X_i remains unchanged. In this way, first, the nmu parameter is defined based on the definition of the mu and the number of variables each time the code is executed. A random number (j) is then determined according to Equation (26), which determines the object function. Finally, using Equation (24), a new value for the selected value is calculated. The sum parameter can also be defined as Equation (27).

$$X_{new,j} = X_j + SUM_j \times rand\left(size_j\right) \tag{24}$$

$$num = \ ceil\ (mu \times nVar) \tag{25}$$

$$j = \ randsample\ (nVar, num) \tag{26}$$

$$sum = 0.1\ (VarMax - VarMin) \tag{27}$$

3.3. Objective function

Recovery coefficient is one of the key parameters in cascade design. When the separation of target isotope is done in several steps, the

Table 2
Concentration of tellurium isotopes in the natural feed.

Number	1	2	3	4	5	6	7	8
Isotope	Te-120	Te-122	Te-123	Te-124	Te-125	Te-126	Te-128	Te-130
Concentration	0.0009	0.0255	0.0089	0.0474	0.0707	0.1884	0.3174	0.3408

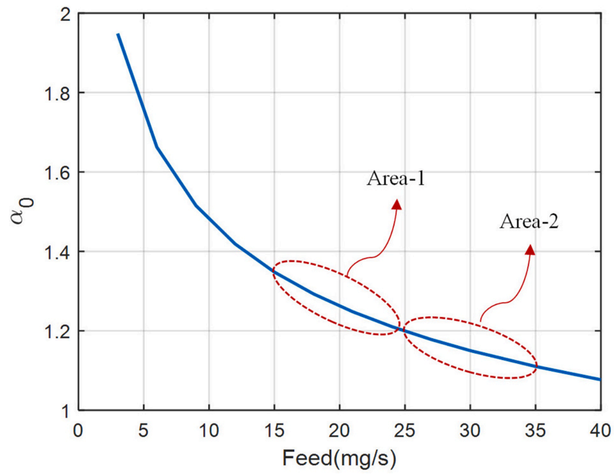

Fig. 3. Separation factor changes in terms of machine feed flow rate.

Table 3
Number of stages and machines in each stage for all the square cascades with 200 centrifuges.

Cascade ID	1	2	3	4	5	6	7
Stage Number	8	10	20	25	40	50	100
Machine/Stage	25	20	10	8	5	4	2

product loss increases and so the recovery coefficient decrease. The higher this parameter, the more product is recovered from the available feed; in other words, the cascade's efficiency has increased. In this regard, how much the amount of waste is reduced, it also contributes to this goal. Moreover, the D function is help to increase the separation of the desired isotope in all steps. For considering these valuable parameters in optimizing and designing cascades, the new objective function can be modified as follow:

$$Object_{Function} = a\frac{1}{Re} + b\frac{1}{D} + \mathrm{c}\ \frac{TotalWaste}{TotalFeed} \tag{28}$$

Subject to:
$C_k \geq 0.65$,
Total Machine $= 200$
that, $Re = \frac{y_{i,P}.P}{z_{i,F}.F}$

The objective function as Equation (28) resulted in the Maximum value of the D and Re considering the specific concentration of target isotope in the product flow, C_k^*. In this regard, the coefficients a, b, and c are selected according to the problem conditions.

4. Material and methods

It could be performed calculations for a certain number of centrifuges to achieve the desired concentration of target isotope (C^*_k). In this paper, the working method is presented as an example for the 200 gas centrifuges and the $C^*_3 = 65$ %. Moreover, natural tellurium hexafluoride gas with eight stable isotopes is used as feed to separate its third isotope (Te-123). The concentration of its isotopes in the natural state are given in Table 2. The components are numbered from isotope 120 to 130 according to their isotopic mass.

As shown in Table 2, the separation of the third isotope is more complicated among the intermediate isotopes. Because this middle component is located between the second and fourth isotopes with much lower concentrations.

Relation (29) is also used to determine α_0, as shown in Fig. 3.

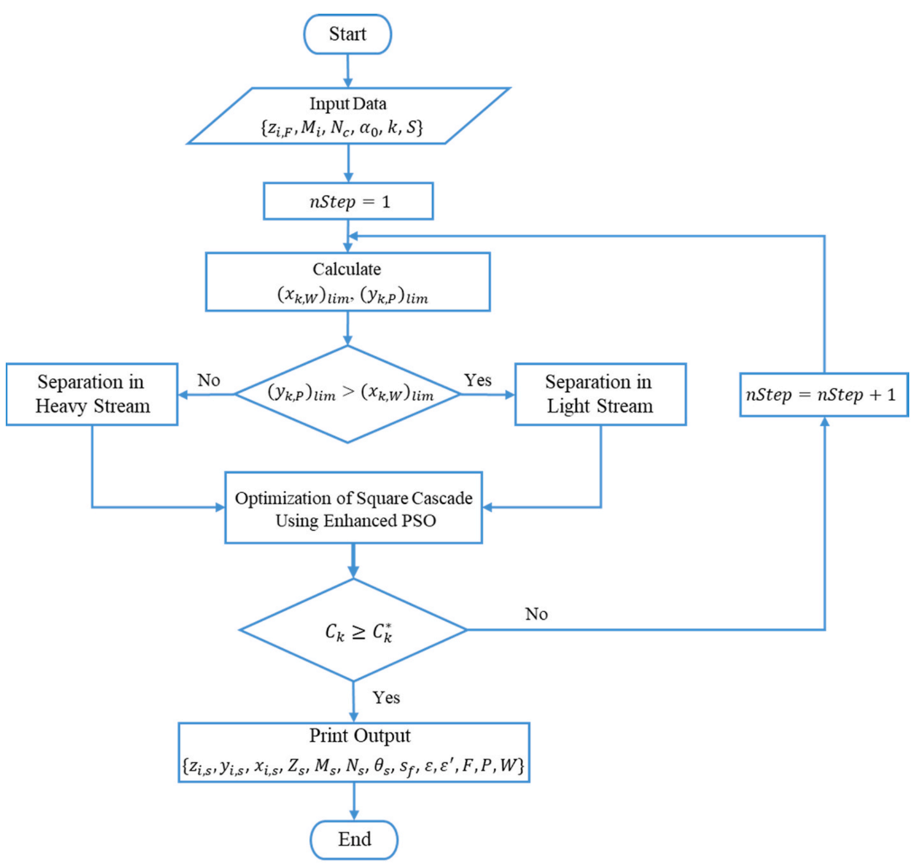

Fig. 4. Algorithm for optimizing cascade parameters by PSO method.

Table 4
The comparison of best solution for cascade obtained by different optimization algorithms.

Optimization Algorithm	ABC [3]	PSO	GWO	WOA	SCA	HS	SSA
$C_{P,Si-28}$	0.9999	0.99990	0.99998	0.99990	0.99998	0.99995	0.99990
$C_{W,Si-28}$	0.01	0.00001	0.00429	0.00546	0.00748	0.00000	0.00089
S	52	52	52	52	52	52	52
$\mathbf{S_F}$	25	32	9	8	10	40	42
$\sum$**Z, (gr/s)**	291.31	260.00	480.43	552.29	329.05	310.30	370.35

$$\alpha_0 = 2.506 * f^{-0.229} \tag{29}$$

In this relation, f(mg/s) is the feed flow rate entering the gas centrifuges. Besides, to better evaluate the results, calculations for the separation factor have been performed in two different ranges:

$$\begin{aligned} &\text{Area}-1:\ if\ 15\frac{mg}{s} < f_{mach} < 25mg\Big/s \rightarrow 1.2 < \alpha_0 < 1.35 \\ &\text{Area}-2:\ if\ 25\frac{mg}{s} < f_{mach} < 35mg\Big/s \rightarrow 1.1 < \alpha_0 < 1.2 \end{aligned} \tag{30}$$

Having the specifications of the gas centrifuge, and the feed properties, the main steps of work are as follows:

a. Specifying the available options for creating a square cascade with 200 machines;
b. Optimization of the above cascades for the separation of the Te-123.

4.1. Specifying the available options to create a square cascade

According to Table 3, the number of possible cascades are 7 for 200 gas centrifuges. Therefore, optimization calculations are performed for these square cascades.

4.2. Optimization procedure

In this research, a code titled "MCSQCA-PSO" has been developed to optimize a flexible square cascade. To find the optimal parameters, the code execution steps are divided into the following sections (Fig. 4): 1) Determining the initial data including the number of stages, centrifuge machine specifications and separation factor, feed characteristics, and target isotope, 2) Determining the path of separation of the square cascade to enter the first step, 3) Optimization of square cascade parameters with enhanced PSO algorithm, 4) Investigation of target isotope concentration in product,C_k, 5) Increase of steps number, nStep, and 6) Determination of flexible square cascade separation path to enter the next step.

Maximum attainable concentration in light or heavy streams may be estimated according to Equations (31) and (32). When the isotope k is enriched in the cascade product (at light end), the maximum extractable concentration is evaluated from Equation (31). When the isotope k is enriched in the cascade waste (at heavy end), Equation (32) assess the maximum extractable concentration [5, 6].

$$\left(y_{k,P}\right)_{lim} = \frac{z_{k,F}}{\sum_{i=1}^{k} z_{i,F}} \tag{31}$$

$$\left(x_{k,W}\right)_{lim} = \frac{z_{k,F}}{\sum_{i=k}^{N_c} z_{i,F}} \tag{32}$$

Therefore, it is specified that the target isotope is separated in the light stream or heavy stream as follow:

$$\begin{aligned} &If\ \left(y_{k,P}\right)_{lim} > \left(x_{k,W}\right)_{lim} \\ &k \rightarrow Light\ Flow \\ &\text{Else} \\ &k \rightarrow Heavy\ Flow \end{aligned} \tag{33}$$

The particle vector consists 5 × nStep arrays. The number 5 is related to the optimization parameters in a square cascade. These parameters are the cut of the first stage, the cascade cut, the feed point, the cascade feed rate, and the machine feed rate. The number of variables increases in proportion to the number of steps when more than 1 step is needed to separate the target isotope. Equation (34) represents a particle in the MCSQCA-PSO. The values of these vectors are generated randomly within the defined range during the optimization calculations.

$$Particle = \left[\theta_{1,S1}, \theta_{Cascade,S1},\ sf_{S1},\ F_{S1}, f_{machine\,S1},\ \theta_{1,S2}, \theta_{Cascade,S2},\ sf_{S2},\ F_{S2}, f_{machine\,S2}, \ldots\right] \tag{34}$$

Having assumed optimization variables for M vectors the particles arrays are randomly selected. Then the flow rates in all stages are determined based on Equations (1)–(13) and the concentrations distribution are calculated according to Equations (14)–(20). So, the fitness of new populations in optimization manner will be calculated and compared with the other populations. Latterly, from among the created

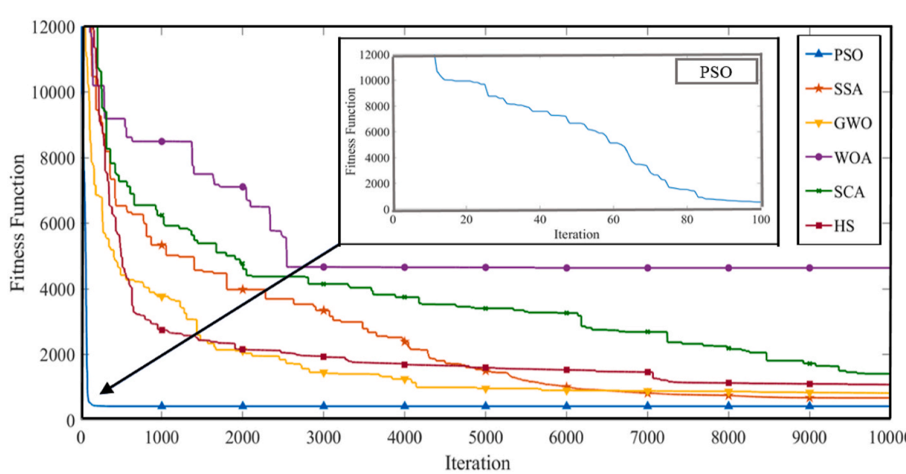

Fig. 5. Fitness function vs. iteration numbers for different optimization algorithms.

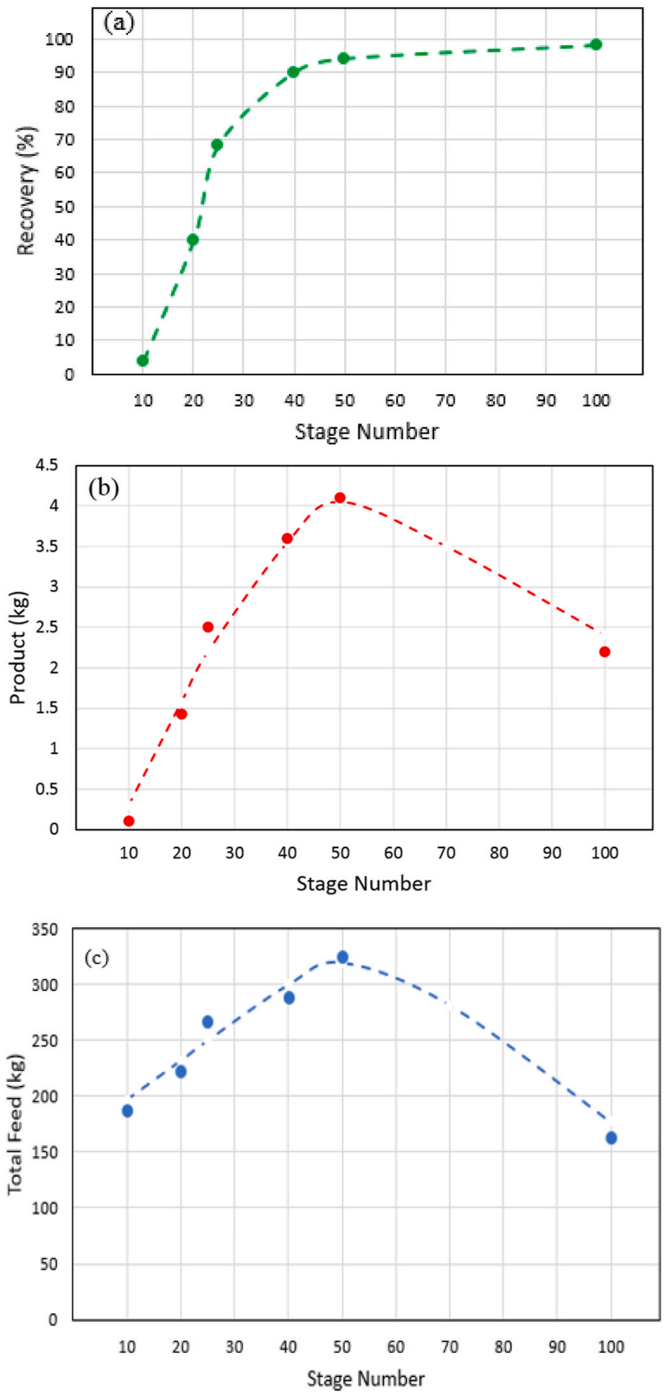

Fig. 6. The amount of feed, product, and recovery of the square cascades for Te-123 separation up to 65 % with lower alpha.

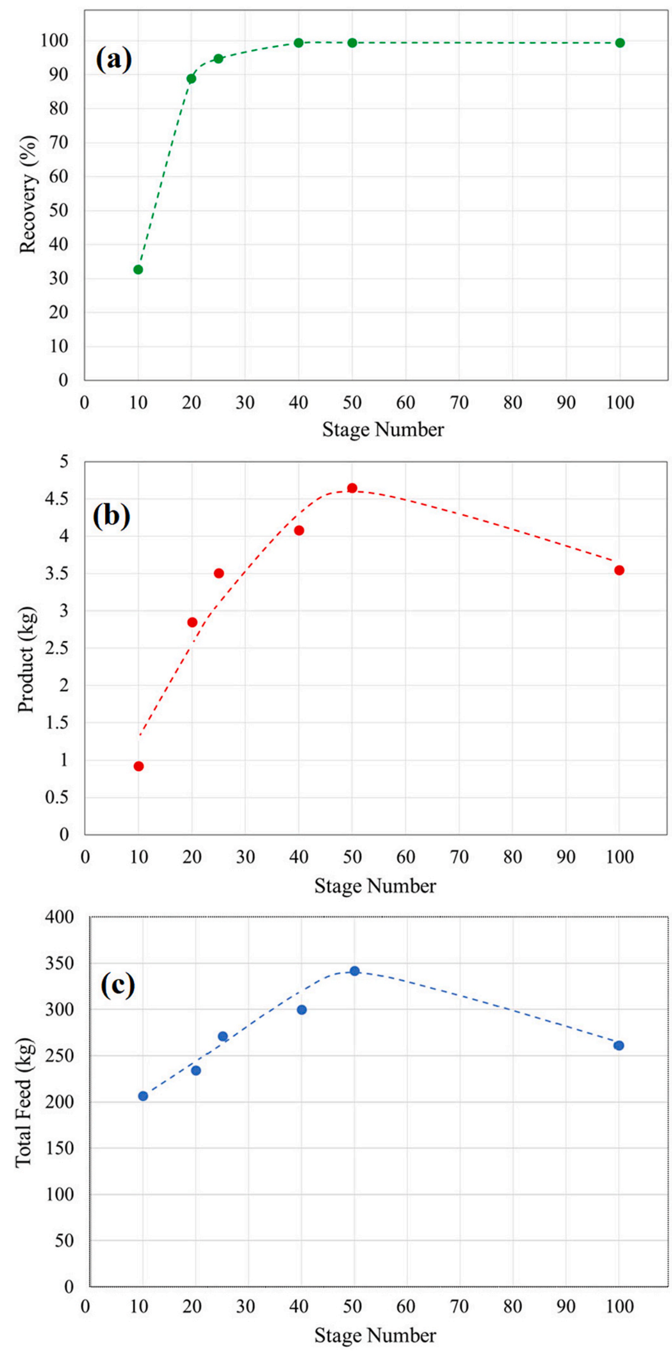

Fig. 7. The amount of feed, product, and recovery of the square cascades for Te-123 separation up to 65 % with high alpha.

vectors new population based on its fitness value is selected and replaced with the initial selected population. This procedure is done based on enhanced PSO as long as the max iteration and the optimization are completed. Various methods have been proposed to determine the concentration of components (Filippov et al., 1992; Wu et al., 1998; Zeng and Ying, 2000b) which uses the Q-iteration method in this study (Zeng and Ying, 2000b).

It should be noted that to improve the optimization solution in this paper, the acceptable ranges of cut in each stage have been considered only between 0.4 and 0.6. If $0.4 < \theta_{1,S}, \theta_{2,S}, \ldots, \theta_{5,S} < 0.6$, the cascade is acceptable; Otherwise, the wrong answer will be removed applying penalty factor. For example, if the cut value exceeds the allowable range, the penalty factor, which is set to 1000 here, removes the wrong answer value from the answers.

5. Results and discussion

In order to demonstrate the capability of the MCSQCA-PSO, and finally to express the method based on it, the results are presented in this section.

5.1. Comparison the results of MCSQCA-PSO with other optimization algorithms

To confirm the validity of proposed code, the results are compared

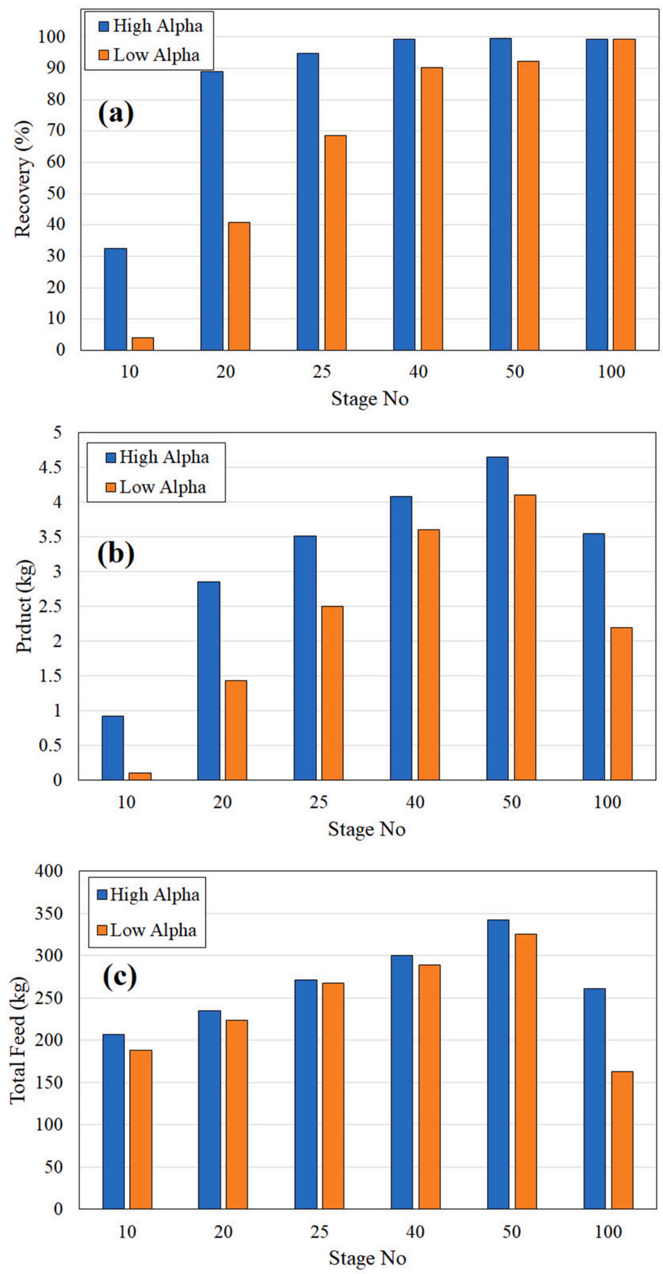

Fig. 8. Comparison of the results with high and low alpha.

with the values reported by Azizov et al.(2020a, 2020b) which used the ABC algorithm for square cascade optimization. Moreover, the results are compared with other optimization algorithms such as HS, GWO, SCA, WOA, and SSA (Geem et al., 2001; Karaboga, 2005; Mirjalili, 2016; Mirjalili et al, 2014, 2017; Mirjalili and Lewis, 2016). It is required to note that, in this comparison PSO is used without the mutation operator.

In this comparison, the product flow of the cascade and the α_0 are considered to be 1 (g/s), and $\sqrt{3}$ as reference (Azizov et al., 2020a, 2020b). Moreover, the minimum and the maximum value of Si-28 in the light ($y^*_{1,P}$) and heavy streams ($x^*_{1,W}$) are also 99.99 % and 0.01 %, respectively. The natural concentration of silicon isotopes (Si-28, Si-29, Si-30) in the feed are 92.31 %, 4.7 %, 3.09 %. The results in Table 4 indicate that the total flow rates ($\sum Z$) obtained by ABC, HS, GWO, SCA, WOA, SSA, algorithms and PSO are about 291.31, 310.30, 480.43, 329.05, 552.29, 370.35 and 260.00 (gr/s), respectively. One can find that PSO reached the optimal parameters of the cascade with better fitness value in comparison with HS, WOA, GWO, SSA, and SCA

Table 5
Feed, product, and recovery of square cascades for Te-123 separation up to 65 % enrichment with lower alpha.

Stage Number	10	20	25	40	50	100
Feed (kg)	187.9	223.4	267.4	288.6	325.4	163.2
Product (kg)	0.100	1.43	2.5	3.6	4.1	2.2
Recovery (%)	0.04	40.75	68.49	90.21	92.38	99.4
$C_{3,1}$	0.1244	0.1670	0.2027	0.2256	0.2275	0.2225
$C_{3,2}$	0.1660	0.2651	0.4705	**0.6515**	**0.6507**	**0.6505**
$C_{3,3}$	0.2327	0.5679	**0.6505**			
$C_{3,4}$	0.3122	**0.6838**				
$C_{3,5}$	0.3820					
$C_{3,6}$	0.4635					
$C_{3,7}$	0.5349					
$C_{3,8}$	0.6062					
$C_{3,9}$	**0.6568**					

algorithms. The results of numerical optimization show that the number of stages from the optimization of the cascade are also close to that of the cascades in reference (Azizov et al., 2020a, 2020b). The values of the ΣZ, $y_{1,P}$, $x_{1,W}$, N, s_f in the corresponding optimized cascades are also shown in Table 4. Due to the good results of MCSQCA-PSO, the PSO can be used as a suitable method for designing the square cascade. It's obvious from Fig. 5 that the PSO algorithm requires fewer iteration for convergence.

5.2. *Optimization results for isotope separation*

This section presents the optimization results for separation of Te-123 over one year. In this regard, the recovery coefficient and the amount of product for square cascades with the number of stages 10, 20, 25, 40, 50, and 100 in two different separation factors are evaluated.

As shown in Figs. 6 and 7, the recovery coefficient increases with increasing the number of stages from 10 to 100. For high separation factor, this parameter varies between 32% and 99 %, but for the smaller separation factor, the changes are between 4 % –99 %. Therefore, one of the ways to increase the product recovery is to increase the number of stages, but if it is too much, it becomes ineffective. For example, for stages more than 40, the recovery coefficient remains almost constant. It can be concluded that increasing the number of stages alone is not enough to increase the enrichment. It is better instead of using a very long cascade; several steps used a cascade with shorter stages, especially when the amount of recovery does not change much. This is due to the impact of parameters such as gas centrifuge feed rate, cascade feed rate, separation factor, stages cut, and cascade cut, which in addition to the number of stages affect the recovery coefficient.

Although the recovery coefficient increases by the number of stages, it cannot be expected that the amount of consumed feed and cascade product will always increase (in case the machines number is constant and the separation specifications are the same in all cascades). According to Figs. 6–8 this issue is independent of the separation factor. As can be seen, the amount of cascade feed and product increases by increasing the number of stages to 50. In contrast, decreases for the cascade with 100 stages. This may be for the following reasons (It should be noted that the explanations are valid for a certain number of gas centrifuges considering the same separation specifications):

a) For the cascades with 40, 50, and 100 stages in both cases study, the separation of Te-123 to 65 % is done in two steps. Since, the number of separation steps is the same in three cascades and on the other side, the number of cascade stages increases, the amount of product is reduced in cascade with stage number 100 and so, its feed is less than the cascade with 50 steps.

b) Another point is the Z/F ratio in the cascade. According to Mansourzadeh et al. (2018); Zeng and Ying (2000a), the higher the Z/F ratio, the higher the separation and performance of the cascade. The number of machines in the short cascades is more, and as a result, parameter Z

Table 6
Feed, product, and recovery of square cascades for Te-123 separation up to 65 % with high alpha.

Stage Number	10	20	25	40	50	100
Feed (kg)	206.9	234.4	271.4	300	341.96	261.2
Product (kg)	0.924	2.85	3.51	4.08	4.65	3.55
Recovery (%)	32.6	88.9	94.69	99.33	99.46	99.4
$C_{3,1}$	0.1687	0.2253	0.2264	0.2225	0.2225	0.2225
$C_{3,2}$	0.3184	**0.6507**	**0.6505**	**0.6500**	**0.6509**	**0.6505**
$C_{3,3}$	0.4880					
$C_{3,4}$	**0.6508**					

becomes high. So, it can be found a cascade with more feed flow rate (F) through optimization calculations. But when the number of cascade stages reaches 100, there are only 2 machines in each stage. Even if the gas centrifuges work at the highest feed rate, the Z/F ratio increases by decreasing F. This leads to reduction in the amount of feed and consequently, the cascade product (Despite having the highest recovery coefficient in the calculations related to the two separation factors).

According to the obtained results, the amount of feed per machines in the cascade with 100 stages is high, and in contrast, this is lower for the cascades with less than 40 stages. In the short cascades, the number of gas centrifuges in each stage is 2–4 times more, and the number of stages is less than half. So, the machines must work with the maximum separation factor and therefore, they have to use the least amount of feed rate. When the number of machines is constant, the shorter cascades become wider and the Z/F ratio increases. According to Equations (10) – (12) the cut changes range reduces and makes it easier to operate the cascade. Also, the important note about the long square cascades is that it is challenging to implement operationally. For example, in a cascade with 100 stages, there are only two centrifuges in each stage, and if one machine crashes, the load falls on the other machine. Also, because a gas centrifuge works with its maximum feed, the amount of separation factor in it reduces, and it may reduce the concentration.

If the separation factor is high, all cascades except the 10-stage cascade would enrich the Te-123 in two steps, and the 10-stage

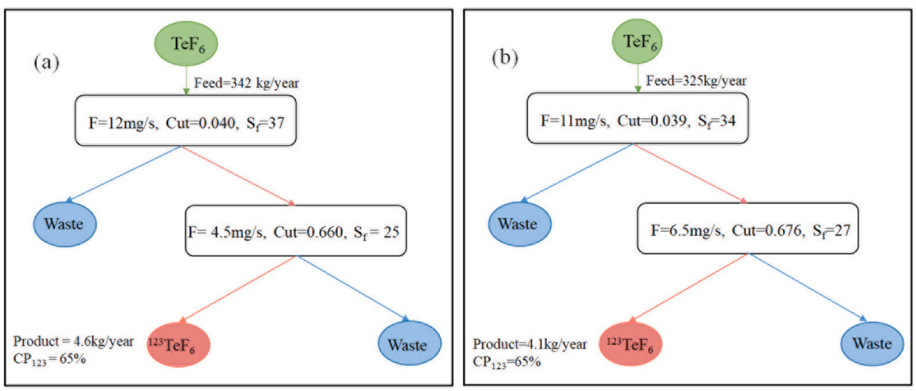

Fig. 9. Te-123 isotope separation path in a square cascade with 50 stages in two states with (a) high separation factor, (b) low separation factor.

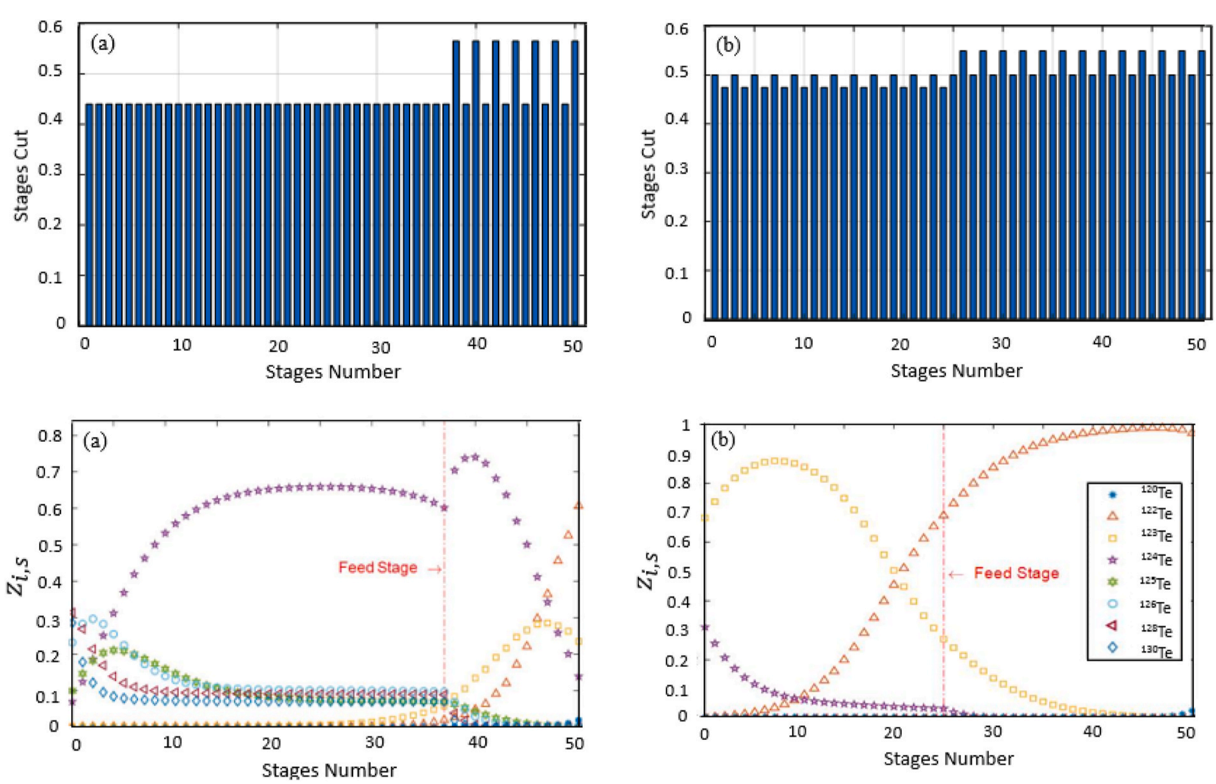

Fig. 10. Isotope concentration and stages cut in a 50-stage cascade with high separation factor, a) the first step, b) the second step.

cascade would enrich through four steps (see Tables 5 and 6). When the separation factor decreases, cascades with 10, 20, and 25 stages need 9, 4, and 3 steps. By increasing the separation factor, the recovery coefficient of cascades increases, and the number of separation steps decreases. In contrast, the number of separation steps increases, and the recovery decreases when the separation factor decreases. Only in the case of a square cascade with 100 stages, the maximum recovery can be expected for the two separation factors. It is necessary to pay attention that, the achievement to 65 % has been desired in this work and if the target isotope concentration changes, the amount of recovery and the number of steps will change.

In Accordance with Fig. 8, the effect of the separation factor on the recovery coefficient and, consequently the amount of product obtained in the low-stages cascade is much more than the high-stages cascade. But the amount of separation factor has little effect on the total cascade feed. This may be because it depends on the structure and shape of the cascade. The feed rate is affected by Z, and the Z/F ratio. But the amount of product in addition to the Z/F ratio is affected by the amount of separation factor. So, the higher the recovery and separation rate, the more product is produced.

Based on the results, investigation among the available options to achieve 65 % enrichment shows the best choice is a cascade with 50 stages. This cascade, in addition to having a high recovery, has the highest amount of feed and product. Fig. 9 is a schematic diagram of the separation route of the Te-123 in two steps for the cascade with 50 stages. As can be seen, in the first step, the desired product exits from the light stream, and in the second step it exits from the heavy stream of the cascade. In this cascade, the desired isotope recovery is equal to 99.46 %, and the amount of feed and product of the cascade is equal to 342 and 4.6 kg, respectively. If the amount of separation factor becomes less, the amount of feed and product is equal to 325 and 4.1 kg, and in this case, the cascade recovery is 92.38 %. Fig. 10 also shows the cut value of the stages and the isotopes' concentration in all stages for a 50-stage cascade with a high separation factor, for two steps.

In practice, after determining the optimal values of the cascade parameters in each separation step, the amount of the feed flow rates entering the machine, the stages cut, the cascade feed rate, and the feed location are adjusted to achieve the specified enrichment value. All of the cut parameters help to determine the flow distribution in the cascade, and by using control valves that are placed among stages, it can be possible to adjust the optimum flow distribution in the cascade. When the flows adjusted as the same for calculation, the concentration distribution of isotope achieved as the calculation expected.

6. Conclusion

In order to design a cascade, it may be necessary to determine its optimal parameters so that the desired isotope separation can be performed in the best possible way. In this regard, a new and efficient code called "MQCSC-PSO" has been developed to optimize the parameters of a flexible square cascade for separation of stable isotopes. In this code:

- The separation of stable isotopes in several steps, using variable separation factor with a certain number of centrifuges have been done.
- The object function with a new approach has been introduced. The highest amount of recovery in the cascade with a certain number of centrifuges was considered as the goal to achieve the desired concentration of target isotope in the product stream. High recovery indicates less feed consumption per production of the same product, which has been investigated for the first time.
- There is no need to define the concentration of the desired isotope in each step using the model cascades. The concentration is calculated and optimized automatically based on the optimization procedure for all steps.
- The particle swarm optimization algorithm was modified using mutation operator and employed to find the optimal parameters of the square cascade.

In order to confirm the validity of the presented scheme, the proposed code was evaluated using the data published in reference (Azizov et al., 2020a) for the separation of silicon in square cascade. Furthermore, the ability of MCSQCA-PSO is evaluated with other optimization algorithms. Suitable alignment of the results indicates that the use of the PSO for this problem guarantees the calculation of the optimal parameters.

Moreover, the square cascade optimization has been conducted for the separation of the 3rd isotope of tellurium. The results show that if the number of stages increases, the recovery coefficient also increases nonlinearly. However, this does not include the amounts of product and required feed. These values reach to a maximum and decrease again due to increasing the stages number. Therefore, it cannot always be expected that the longer cascade is the best option to choose, in comparison with the others. Furthermore, the shorter cascades become wider, and this not only increments the amount of feed and capacity of the cascade by increasing the Z/F ratio, but also makes the stages cut with less change than each other. This issue is important in the operational cascade. In addition, according to the obtained results, increasing the separation factor has a significant effect on the amount of product and recovery coefficient in the shorter cascades. But it does not have much effect on the amount of required feed.

In this research, studies were performed for the cascades with 200 gas centrifuges and the number of stages was considered between 10 and 100. According to the results, the cascade with 50 stages is the best option for separating the third isotope of tellurium (Te-123). In this cascade, the desired isotope recovery is equal to 99.46 %, and the amount of feed and product of the cascade is equal to 342 and 4.6 kg, respectively. If the amount of separation factor becomes less, the amount of feed and product is equal to 325 and 4.1 kg, and in this case, the cascade recovery is 92.38 %.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Glossary

α_0: unit separation factor [-]
θ_n: Stages cut [-]
M: Molar mass gr/mol
$\theta_{Cascade}$: Cascade cut [-]
s: Number of stages [-]
s_f: Feed stage [-]
F_{mach}: Machine feed flow rate mg/s
F: Cascade feed flow rate mg/s
$z_{i,F}$: Feed concentration [-]
P: The light cascade product mg/s
W: The heavy cascade product mg/s
Z_n: Input feed rates to stages mg/s
M_n: Up flow rate of stage mg/s
N_n: Down flow rate of stage mg/s
ε': Flow rate back to the last stage mg/s
ε: Flow rate back to the first stage [-]
$w_{i,n}$: Mole or mass fraction of components in the heavy cascade product [-]
$y_{i,n}$: Mole or mass fraction of components in the light cascade product [-]
$z_{i,n}$: Mole or mass fraction of components in the cascade feed [-]
D: Two-group parameter [-]
C_k^*: The desired concentration of the target isotope [-]
C_k: Target isotope concentration at the end of each step [-]