Optimization of cascades with variable overall separation factors by various efficiency criteria

G A Sulaberidze¹, A P Mustafin¹, A Yu Smirnov¹, V D Borisevich¹, S Zeng² and D Jiang²

¹ National Research Nuclear University MEPhI, 31 Kashirskoe Shosse, Moscow 115409, Russian Federation
²Tsinghua University, Department of Engineering Physics Beijing 100084, P.R.China

Abstract. Construction and operation of separation facilities require considerable investments. That is why the special attention in the theory of isotope separation in cascades is paid to their optimization. The installation allowing obtaining the required quantity of a commercial isotope product by a minimum unit cost it is customary to call as the optimum cascade. However, the use of such the criterion in theoretical calculations is inconvenient, in view of the fact that the cost coefficients are generally inaccessible and can vary depending on external factors. Therefore, theoretically the minimum possible number of separation unit or elements, for instance, gas centrifuges, is often used as the optimization criterion, since its value directly indicates the unit costs. In addition, such criteria as the minimum of the total cascade separation capacity or the minimum of the deviation sums of the maximum possible separation capabilities are also applied in the optimization calculation. In this connection for the case of the cascade with a variable from stage to stage overall separation factor of a centrifuge, the parameters of the cascades optimized by means of various optimization criteria may differ largely. In this paper, we compare the parameters of cascades with the same external conditions, which are optimized by the above criteria. As the criterion to compare all cascades under investigation is chosen the minimum number of separation elements in the installation. The chosen approach allows us to estimate the deviation in the number of gas centrifuge in a case of optimization of a separation plant by different efficiency criteria.

1. Introduction

As is well known, for separation of isotopes in cascades of gas centrifuges, one of the key criteria for determining the efficiency of such an installation is the minimum financial cost for obtaining the required product. However, in view of the specifics of the nuclear industry, it is not always possible and expedient to use the minimum of financial costs as a criterion in theoretical studies devoted to optimization of separation processes in cascades of gas centrifuges (GC) [1]. Therefore, other criteria that indirectly determine financial costs are often applied. One of these quantities is the total number of separation elements (centrifuges) in the cascade [2], since it basically determines the unit costs for obtaining the isotope product.

In the theory of cascades it is proved that if the separation factor of a single separation element depends only on a feed flow (capacity), then the number of separation elements in the cascade is directly proportional to its total flow, and for the same performance of all elements at cascade stages, the criterion of the minimum separation elements in the cascade and the minimum of the total flow in a cascade coincide. Assuming that all cascade elements are identical and operate in identical mode, the
total number of separation elements is directly proportional to the value of the total flow in a cascade. Therefore, often in calculation proceed from the minimum of the total flow as a criterion for cascade [3]. However, the use of the total flow as a criterion is justified only in the case of identical operating modes of the elements. In the case of variable overall separation factors and cuts at cascade stages of the use of this criterion may lead to errors in the calculation of the optimal parameters [4]. That is why in the works of some researchers it was suggested to use other efficiency criteria. For example, in [5], when optimizing the cascade of centrifuges, the criterion of the minimum of the deviations for the separative powers of cascade stage stages from their maximum possible values was used. In this regard, it is necessary to analyze this criterion in order to determine its place among many others, as well as to indicate the limits of its applicability. The results of such studies are called up, in many ways, to dot the “i” in the question of choosing the correct criteria for optimization of cascades with variable overall separation factors that depend on the parameters of a single centrifuge machine.

The purpose of this research is to develop a technique to optimize a cascade with variable separation factors at its stages and as well as comparison of the cascade parameters optimized by means of various efficiency criteria reviewed in this study. The efficiency of various criteria is defined by comparison with the results obtained by optimization procedure using the total number of separation elements as the efficiency criterion.

2. Description of the cascade model
As the object of research a symmetrical countercurrent cascade for uranium enrichment is considered (Figure 1). The working substance is uranium hexafluoride (UF₆) [6-7].

![Figure 1. Schematic drawing of the symmetric countercurrent cascade](image)

The external parameters of a cascade are the following variables that determine the external operating conditions: \( F, P, W \) are the feed, product, and waste flows in the cascade, respectively; \( C_{IF}, C_{IP}, C_{IW} \) are the concentrations of the components in the these flows. The internal parameters include: \( N \)th total number of stages in the cascade; \( f \) is the number of the stage, where the feed flow enters the cascade; the parameters of the stages are as follows: \( L_s, L_s', L_s'' \) are one input and two output flows at the \( s \)th stage of the cascade; \( C_{iF}, C_{iP}, C_{iW} \) are the component concentrations in the corresponding flows; the overall separation factor and separation factors of enriching and depletion sections at the \( s \)th stage of the cascade \( \beta_s, \alpha_s, \beta_s' \) and the corresponding cuts at cascade stages \( \theta_s \) (\( s=1,2...N \)).

In the absence of losses of the working substance at cascade stages and in the stationary mode of cascade operation, the external parameters must satisfy the equations of the material balance equation:

\[
F = P + W, \quad (1)
\]

\[
FC_{iF} = PC_{iP} + WC_{iW} , \quad i = 1,2,...,m. \quad (2)
\]
The internal parameters of the stage with the number \( s \) \( (L_s, L_s', L_s'', C_s, C_s', C_s^\prime) \) in the stationary mode of the cascade, in the absence of losses of the working substance at the stages of the cascade, are related by the equations of the balance of matter and each component: for the enrichment part of the cascade

\[
\theta_j L_s - (1 - \theta_{s+1}) L_{s+1} = P,
\]

\[
G'_{i,s} - G''_{i,s+1} = PC_{iP} ,
\]

for the depletion part of the cascade

\[
\theta_j L_s - (1 - \theta_{s+1}) L_{s+1} = -W,
\]

\[
G'_{i,s} - G''_{i,s+1} = -WC_{iW} .
\]

The external and internal parameters of the cascade are connected by the following boundary conditions

\[
L'_{N} = \theta_N L_{N} = P ,
\]

\[
L''_{1} = (1 - \theta_1) L_1 = W ,
\]

\[
C'_{N} = C_{iP} ,
\]

\[
C''_{1} = C_{iW}, i = 1,2,...,m.
\]

To calculate the cascade parameters, it is necessary to specify the separation characteristics of a stages. As a rule, they are expressed in the form of dependencies:

\[
q_s = q_s(\theta_j, g_s),
\]

where \( q_s \) is the overall separation factor of a stage with the number \( s \), \( g_s \) is the a feed flow to a single separation element in a stage \( s \), and \( \theta_j \) is a cut at a cascade stage with the number \( s \) \( (\theta_j = L'_j/L_j) \). A similar dependence of the separation factor is due to the independence of isotopic composition observed for kinetic methods of separation [8-9].

In the case of a binary mixture \( (m = 2) \), for each stage with the number \( s \) one can find the concentrations \( C'_s, C''_s \), according to formulas

\[
C'_s = \frac{q_s C''_s}{1 + (q_s - 1) C''_s} ,
\]

\[
C''_s = \left(1 - \frac{r'_s}{G'_s}\right) + \frac{r''_s}{G''_s} ,
\]

where \( r'_s \) and \( r''_s \) are the transit flows of a separated mixture and a target isotope in the direction of the cascade waste flow, that are equal to \( r'_s = W, r''_s = WC_w \) for \( s < f, r'_s = -P, r''_s = -PC_p \) for \( f < s < N \).

The task of cascade optimization is formulated as the definition of the internal parameters that minimize the selected effectiveness criterion on a set of acceptable values, with the selected external parameters satisfying the condition \( C'_N = C_p, C''_1 = C_w \). As an example it can be the total number of separating elements (in the case under review these are gas centrifuges), \( \gamma = \sum Z_s \rightarrow \min \).

To obtain the desired equations, it is assumed that the number of gas centrifuges in the first stage \( Z_1 \) is defined as an implicit function of the quantities \( Z_1, ..., L_2, ... , L_N \), and then the extreme condition of the function is written \( \gamma \).

For the closure of the system of equations (1) - (13), it is necessary to know the dependence of \( q_s \) on a feed flow \( g_s \) to a centrifuge and on the cut \( \theta_j \), which can differ from one to another. The present paper uses the dependence \( q_s = q_s(\theta_j, g_s) \) proposed in [9]:

\[
PCPAS 2017 IOP Publishing
IOP Conf. Series: Journal of Physics: Conf. Series 1099 (2018) 012009 doi:10.1088/1742-6596/1099/1/012009
\]
\[ q = \exp(a_0 + a_1 \theta - a_2 \theta^2) g^{-a_3}, \]  
\text{(14)}

where \( a_0=1.2, a_1=1.8, a_2=2.2 \) and \( a_3=0.4; \), \( g \) (\text{mg} / \text{s}) is the flow of UF_6 to single gas centrifuge. Since the case of obtaining low-enriched uranium from natural raw materials was considered, a formula corresponding to the condition \( C << 1 \) \[10\] was used to calculate the centrifuge separation capacity:

\[ \delta U = g \cdot \left[ \ln(1 + \theta(q - 1)) - \theta \ln g \right]. \]  
\text{(15)}

3. Method of optimization

In view of the fact that the optimization problem being solved is a task of multi-parametric optimization, since a large number of quantities act as parameters in its solution. The latter increases in proportion to the number of stages, what make us carefully choose the optimization method. Within the framework of the work, the genetic algorithm (GA) has been chosen as the optimization method. The main reason for that is as follows. A GA is sufficiently universal and can be suitable for solving a wide class of problems, and also allows us to reduce the calculation time with respect to traditional methods based on quadratic programming. As is known, a GA is one of the methods for solving optimization problems, using an abstract version of evolutionary processes to develop solutions of such problems. Using the terminology adapted to the theory of a GA, let us briefly explain the principle of their realization. Each GA works on a "population" of artificial "chromosomes." These are strings in the final alphabet (usually binary). Each a chromosome is a solution to the problem and has "suitability" is a number that is a measure of how close the solution is to the optimum \[11\]. Below is a brief review of the methodology for solving the problem, implemented on the basis of a GA.

The solution is encoded in the form of a vector ("genome") \text{(16)}, where the first \( N \) numbers are the cuts of the flow at each cascade stage, and the next \( N \) numbers are the feed flows to the separation elements at each stage (where \( N \) is the number of stages in the cascade)

\[ Ch = \{ \theta_1, \theta_2, ..., \theta_N, g_1, g_2, ..., g_N \}. \]  
\text{(16)}

At the first step, a set of vectors ("population") is created randomly. Then, the cascade parameters are calculated and the value by which the cascade is optimized for each set of vectors. The vectors that do not correspond to the boundary conditions are removed and replaced by new ones. Further, all vectors are sorted according to the magnitude of the increase of the optimized value. Then, using the crossovers function, all genomes are sequentially crossed, while the same genomes do not cross.

3.1. Crossover function:

The work uses a modification of the genetic algorithm, in which the crossovers function is combined with the mutation function. In other words, each gene is assigned a number from 0 to 1. If the number is in the range from 0 to 0.2, the new genome receives the gene from the first parent unchanged \text{(17)}

\[ T_{cross}^{i+1} = T_i^p, \]  
\text{(17)}

in the range from 0.2 to 0.4 from the second parent \text{(18)}.

\[ T_{cross}^{i+1} = T_i^q. \]  
\text{(18)}

In the case when the number is in the interval from 0.4 to 0.8, the crossing of the genomes takes place according to formula \text{(19)},

\[ T_{cross}^{i+1} = \frac{T_i^p + T_i^q}{2}. \]  
\text{(19)}

0.8 to 1 new gene is selected randomly \text{(20)}
Then for the genomes obtained, the internal parameters of the cascade and the value of the "fitness function" (suitability function), on which optimization is performed, are calculated. Further, all genomes are sorted according to the magnitude of the optimized value increase and the destruction of genomes with the least suitable value of the optimized value to the amount of the original population. This process is repeated a certain number of times. The more the number of iterations completed, the more accurate the data are obtained. In the case where the difference between genomes is less than a given value, 90% of the population with the worst value of the optimized value is destroyed, and new ones are created randomly instead of the destroyed genomes. Figure 2 schematically shows all the main steps of the genetic algorithm.

\[ T_{\text{cross}}^{t+1} = \text{Rand} \]  

Figure 2. Diagram explaining how the genetic algorithm works

4. Results and discussion
The described algorithm was applied to the above optimization problem of a cascade with variable overall separation factors. Approbation of the algorithm was carried out using cascade optimization for enrichment of natural uranium in the form of uranium hexafluoride (UF₆). The concentration of the target isotope $^{235}\text{U}$ in the product flow is assumed equal to 3%, in the waste flow concentration of this component is taken equal to 0.3%. The product flow is 1 g/s. The number of stages in cascade is five, the feed flow is entered into the second stage. For this set of parameters, the data on the optimal parameters of such a cascade are available in [4, 9], which made it possible to check the developed algorithm. As can be seen, from Table 1, the results showed a satisfactory match in optimizing such a separation stage by the criterion of the minimum number of separation elements at variable coefficients of cascade stage, since the difference in the values given in the Table is less than 0.2%.
Table 1. Comparison of cascade optimization results by the total number of separation elements for different optimization methods

| Optimization method 1 from [12] | Optimization by the SQP method from [12] | Optimization by a genetic algorithm |
|----------------------------------|------------------------------------------|------------------------------------|
| Total number of separation elements | 6352                                      | 6355                               | 6363                               |

Then, optimization was performed using several optimization criteria for a cascade of the same configuration. Namely, the total number of separation elements:

1) $$Z = \sum_{i}^{N} Z_{i}$$ is the criterion characterizing the amount of unit costs for production of isotope product of necessary quality

Optimization of the cascade parameters by the total flow:

2) $$L = \sum_{i}^{N} L_{i}$$ is the criterion for the case of the constant overall separation factors at cascade stages. This criterion is equivalent to the total number of separation elements.

Deviation from the maximum separation capacity:

3) $$\Psi = \frac{\sum_{i}^{N} Z_{i} * (\delta U_{\text{max}} - \delta U_{i})}{\sum_{i}^{N} Z_{i} * \delta U_{\text{max}}}$$ is the criterion characterizing the efficiency of the separation element taking into account the deviation of the relative sum of separation capacities stages from its maximum possible value [5].

The total relative deviation from the maximum separation ability:

4) $$\chi = \frac{\sum_{i}^{N} Z_{i} * (\delta U_{\text{max}} - \delta U_{i})}{\delta U_{\text{max}}}$$ is the criterion which characterizes vicinity of the separation capacity of centrifuges at each cascade stage to their maximum possible value. This takes into account the number of elements at each stage, thus excluding the effect of the number of separation elements on the absolute values of the deviation of the separation capacity from the maximum value [12].

The results of optimization are presented in Table 2 (the parameters corresponding $$\Psi$$ to are multiplied into $$10^{-5}$$ by the order of magnitude of the remaining parameters).
Table 2. Results of optimization by various efficiency criteria

| Basic parameters | Criteria of optimization | $\sum Z_s \rightarrow \min$ | $\Psi \rightarrow \min$ | $\sum L \rightarrow \min$ | $\chi \rightarrow \min$ |
|------------------|--------------------------|-----------------------------|--------------------------|--------------------------|--------------------------|
| $\sum Z_s$       |                          | 6363                        | 6385                     | 6776                     | 6378                     |
| $\Delta U$ mg/s  |                          | 3429                        | 3449                     | 3440                     | 3446                     |
| $\sum L_s$, g/s  |                          | 43.71                       | 44.56                    | 34.13                    | 44.79                    |
| $\Psi \cdot 10^{-5}$ |                        | 272                         | 23                       | 6051                     | 26                       |

$\Delta U$ is calculated as the difference between $\delta U_{\text{max}}$ and the value of $\delta U$, calculated for each step.

From the analysis of the obtained data it follows that for the criteria of the minimum of separation elements and the minimum of the total deviation from the maximum separation capacity, the difference in the total number of centrifuges is less than 0.4%, for a total separation capacity of less than 0.8%, and for a total flow of about 5%. It can be explained by the fact that all three criteria actually characterize the efficiency of using a single separation element in a cascade, so the optimal parameters for these cases turned out to be quite close. However, it is important to note the fact that in the case of optimization of the cascade by the smallest number of separation elements, the total deviation of the separation capabilities of the stages was not minimal. This means that in terms of cascade optimization, it is not necessary to work at maximum separating ability for each single separation elements in the cascade. As for optimization in the minimum of the total cascade flow in a cascade, it can be seen that the difference in the total number of centrifuges is much larger than for all others optimization criteria, what is more than 6%. Consequently, as a criterion of optimization of the cascade within the framework of the task under investigation, it cannot be used, since the obtained cascade parameters will not provide the minimum unit costs for obtaining the desired isotope product.

To verify the "generality" of the above conclusions, an additional series of calculation of the optimum parameters of the cascade for enrichment of $^{235}\text{U}$ to 5% from the natural abundance with a 0.3% in a waste flow was carried out. The product flow is 1 g / s. The total number of stages in the cascade is equal eight. A feed flow goes to the third stage. The number of stages in the cascade and the number for a feed flow stage were estimated using the ideal cascade model. The optimization results are presented in Table 3.

Table 3. Results of optimization by various criteria, obtained using the genetic algorithm

| Basic parameters | Criteria of optimization | $\sum Z_s \rightarrow \min$ | $\Psi \rightarrow \min$ | $\sum L \rightarrow \min$ | $\chi \rightarrow \min$ |
|------------------|--------------------------|-----------------------------|--------------------------|--------------------------|--------------------------|
| $\sum Z_s$       |                          | 14006                       | 15136                    | 15250                    | 14111                    |
| $\Delta U$ mg/s  |                          | 7254                        | 7852                     | 7564                     | 7289                     |
| $\sum L_s$, g/s  |                          | 134.35                      | 126.39                   | 110.40                   | 131.31                   |
| $\Psi \cdot 10^{-5}$ |                        | 4154                        | 3997                     | 8205                     | 4410                     |
As one can see the exact total number of separation elements, the total separation capacity, the deviation from the total separation capacity, the total flow and the total relative deviation from the possible maximum separation ability, for each criterion the deviation in the number of separation elements from the number of separation elements obtained by the criterion of the total number of separation elements is 21.19%, 7.47%, 8.16%, 0.74%, respectively. Thus, we can conclude the regularities inherent in the previous case are also fulfilled qualitatively in this example as well. However, the absolute values of the discrepancy in the set of parameters obtained by my means of various criteria have increased. The latter can be explained by an increase in the total number of stages in the cascade.

5. Conclusion
In this paper, we propose a method of optimization of a symmetric countercurrent cascade with variable separation factors at its stages obtained by various efficiency criteria, i.e. the minimum number of separation elements, the minimum of the total flow and the minimum deviation from the maximum of the separation ability based on the genetic algorithm. With the use of the developed technique, computational experiments were carried out on optimization of the cascade parameters for enriching natural uranium under the condition of the variable overall separation factors at cascade stages and usage of various efficiency criteria. The analysis of the obtained results showed that the difference in the number of separation elements (and, consequently, unit costs) for a given task when using the number of separation elements and deviation from the maximum of the separation ability as a criterion is relatively small and does not exceed fractions of a percent. Wherein, the difference in the case of optimization in the total flow reaches several percent. Moreover, the minimum value of the total flow does not correspond to the case of the minimum number of separation elements, which indicates that the total flow cannot be used as an optimization criterion in cascades with variable separation coefficients.

Acknowledgments
This research is supported by Natural Science Foundation of China (Grant No. 11575097), the National Key Basic Research and Development Program of China (Grant No. 2014CB744100), and the Sino-Russian joint project from National Natural Science Foundation of China (Grant No. 1151101155) and Russian Fund for Basic Research (Grant No. 16-58-53058 GFEN_a).

6. References
[1] Borisevich V.D. et al. Physical backgrounds of isotope separation by gas centrifuge. MEI Publishing House, 2011.
[2] Cohen K., The theory of isotope separation as applied to the large-scale production of U-235, N.Y., McGraw-Hill, 1951.
[3] Smirnov A.Yu., Borisevich V.D., Sulaberidze G.A., Evaluation of specific cost of obtainment of lead-208 isotope by gas centrifuges using various raw materials, Theor. Found. Chem. Eng. 2012. 46 (4). P. 373-378.
[4] Sulaberidze G.A., Zeng S., Smirnov A.Yu., Bonarev A.K., Borisevich V.D., Jiang D. Efficiency criteria for optimization of separation cascades for uranium enrichment. Nuclear Engineering and Technology. 2018. V. 50. P. 126-131.
[5] Delbeke J.F.A. Theoretical analysis to assess the separative power of reconfigured cascades of predesigned gas centrifuges. Ind. Eng. Chem. Res., 2009, v.48, pp.4960-4965.
[6] Orlov A.A., Tsimbalyuk A.F., Malyugin R.V. Desublimation for Purification and Transporting UF6: Process Description and Modeling, Separation and Purification Reviews. 2017. 46(1). P. 81-89.
[7] Orlov A.A., Tsimbalyuk A.F., Malyugin R.V., Glazunov A.A. Dynamics of UF 6 Desublimation with the Influence of Tank Geometry for Various Coolant Temperature, MATEC Web of Conferences. 2016. 72:01079
[8] Palkin V.A. Optimization of a cascade with arbitrary specified separation coefficients of the stages, Atomic energy. 1997. V. 82. No. 4. P. 190-195.
[9] Palkin V.A. Determination of the optimal parameters of a cascade of gas centrifuges, *Atomic energy*. 1998. V. 84. No. 3. P. 246-253.

[10] Sulaberidze G.A, Borisevich V.D. Application limits of the classical concepts “separation potential” and “separative power” *Atomic Energy*. 2013. 114(6). P.412-420.

[11] M. Mitchell, An Introduction to Genetic Algorithms, *MIT Press*, Cambridge, MA, 1998.