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A new algorithm for simulation of the functional symmetric and asymmetric cascades

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ABSTRACT

Design of cascade based on operational functions of a single machine is an important goal in the isotope separation theory. By recognizing the behavior of gas in a centrifuge machine, a cascade with desirable properties and parameters can be designed. In the classical theory of multistage separation installation, it has been shown that in an ideal cascade (no mixing) the total number of separation elements flow is minimal, and accordingly, the maximum separation work unit (SWU) of the cascade occurs. In the practical form, the cut and separation factors may assume to be dependent on the feed flow. Using specific functional parameters, the algorithm, design the functional cascades (DFUNCAS), can design the functional symmetric and asymmetric cascades. DFUNCAS can design a cascade with stated waste and product concentration. Furthermore, the program can design symmetric and asymmetric cascades. In this work, four test cases were considered and the results show that the DFUNCAS can design any kind of cascade accurately.

Keywords: Algorithm, Cascade, Asymmetric, Symmetric, Design

I. INTRODUCTION

The main part of an isotope separation plant is a separating element in which the feeding material is fractionated to be enriched in the desired and depleted isotopes in the head and tail sections respectively. The centrifuge is one of the most important separating elements that countercurrent flow profile establishes in it and plays an important role in separation isotopes [1-5]. The operational functions of the gas centrifuge play an important role in the cascade behavior and many investigations have been published in this field

[6-8]. The number of stages, size of a stage, product, and waste throughput is dependent on the functional parameters of a single machine [6]. Geldenhuys used the linear algebra method in the design of asymmetric cascades for isotope enrichment [7]. Wood et al. used pancake computer code to optimize and determine the influence of feed rate on separation factors [8-9]. Hu J. et al. proposed a purely axial flow analytical solution and determine the dependence of α on feed [10]. Palkin presented the dependence of α to two

variables θ and feed as a correlation and illustrated that the total number of centrifuges in the ideal cascade is higher than in the optimal cascade [11]. Norouzi et al. presented a realistic function for separation factor in relation to two variables cut, and feed flow rate and determined optimal parameters, α , θ , and feed [12]. Palkin and Igoshin proposed a method for calculating and optimizing a cascade of gas centrifuges with an arbitrary scheme in which cut is an independent quantity and separation factor is dependent on cut and feed flow rate [13]. Borosevich et al. proposed that it is possible to find the optimum parameters of a cascade that operates in the minimum total flow. In this paper, we proposed a new algorithm to design functional symmetric and asymmetric cascades with two correlations that define gas centrifuge characteristics [14]. In the separation unit, among five variables α , θ , β , γ , and Cf, three variables are independent [13]. The feed concentration, Cf, has a low effect on the other parameters in low enriched uranium; however, it can be achieved from the desired mass balance equation in the merging points in the cascade, so only two of the five variables have remained. To approximate the theoretical or experimental points by a simple function, we can state that two parameters in the gas centrifuge, enriching factor and depleting factor, are the functions of feed. In fact, in the gas centrifuge if the cut depends on feed, the proposed equations by palkin will decrease to one variable (feed flow), and for solving or simulating this type of cascades we should have two functions [13]. The objective of this paper is to propose a new algorithm to design a cascade. So first the cascade equations are presented and then the design algorithm is proposed. The design algorithm is divided into two parts: a simulator part and a compression method. The simulator part is connected to the compression method which calculates the stage number of the cascade.

II. CASCADE STRUCTURE AND GOVERNING EQUATIONS

A simple separation cascade consisting of separating units connected in series is shown in Fig. 1. The headstream of a stage goes to feed the next upper stage and its tail stream is recycled at the inlet of the next lower stage [12]. The cascade receives a feeding material, with a molar flow rate F(g/h) and composition XF, and delivers a product stream, with molar flow rate P and composition XP and waste stream with molar flow rate W and composition Xw.

Each centrifuge receives a feed of composition X with flow rate f mole/sec and delivers a product stream of composition X with flow rate f and a waste stream of composition X along flow rate f mole/sec. Stages are sequential numbered from one to N. The cut of machine and separation factors are defined as:

$$\theta = \frac{f'}{f},\tag{1}$$

$$\beta = \frac{X'/(1-X')}{X/(1-X)},\tag{2}$$

$$\gamma = \frac{X / (1 - X)}{X'' / (1 - X'')},\tag{3}$$

$$\alpha = \gamma \beta.$$
 (4)

These four external parameters vary with feed flow rate and this reality leads to optimal cascade design. External parameters must satisfy balances on material and on the desired component over the throughout cascade [15], that is:

$$F = P + W (5)$$

$$FX_F = PX_P + WX_W. ag{6}$$

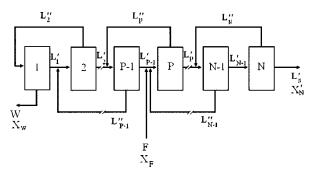


Fig. 1. Cascade of centrifuge with N stages

Internal parameters in the cascade are flow rates and compositions of feed, head, and tail of each stage as well as the total number of stages. The internal parameters of the cascade are determined as functions of the stage equation, taking into account external parameters. In a symmetric cascade with N stages and having θ s for every stage, the flow rate of pipes can be obtained by the following set of material balance equations:

$$L' = \theta_s L_s, \qquad s = 1, ..., N \tag{7}$$

$$L_s'' = (1 - \theta_s)L_s, \quad s = 1,...,N$$
 (8)

$$L_{s+1}'' = L_s' + L_{s+1}'', s = 1,...,N-2, s \neq p$$
 (9)

$$L_{N} = L'_{N+1}, (10)$$

$$L_s = L'_{s-1} + L''_{s+1} + F, \quad for \quad s = p$$
 (11)

$$L_1 = L_2''. \tag{12}$$

where Ls, Ls', and Ls" are the input flow rate, product, and waste stream of an arbitrary stage, respectively. The separation parameters may be expressed in terms of cut and feed. This leads to the design of an optimal cascade [13]. As mentioned above, in the gas centrifuge if the cut depends on feed, the proposed equations changed to one variable and two functions: one function is for separation factor and the second for the dependence of cut on feed. From the mass balance we have:

$$\theta = \frac{(\beta - 1)\left[1 + (\gamma - 1)C_{\gamma}\right]}{\gamma\beta - 1},\tag{13}$$

So, the second function may be expressed as a function of β or γ on feed.

In the separation of isotope mixtures, the cost of work is the biggest part of the price of the enriched material. For the series of isotope separation methods, these costs can be estimated from separative power. For a plant with a single tail, product, and feed stream the separative power is given by:

$$\delta U = WV(x_w) + PV(x_p) - FV(x_f),$$

$$V(x) = (2x - 1)Ln \frac{x}{1 - x}.$$
(14)

The non-ideality in centrifuge cascade can define by:

Non - identity = (SWU of cascade - SWU of total stage) / SWU of cascade

III. PROPOSED CASCADE DESIGN ALGORITHM

Design of the separation cascade accomplished with distinguished parameters (single machine characteristic, flow rate, and concentration of feed, waste, and product). The waste and product streams (W and P) are expressed by the mole fractions of xw and yp. Figure 2 shows the logic of the algorithm that used in the design of the separation cascade. In the first step, the initial data is given. There is a calculation core in the second step that is illustrated in Fig. 3. In the third step if y<yp and x>xw, one stage is added to the product and the waste, and the algorithm goes to the second step. In the fourth step, if $y \ge yp$ and $x \ge xw$, one stage is added to waste, and the algorithm goes to the second step. In the fifth step, if y<yp and x=<xw, one stage is added to the product, and the algorithm goes to the second step. Also, this algorithm has a core calculation that calculates the θ of each stage.

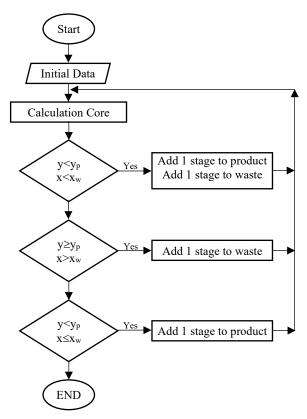


Fig. 2. The procedure of determining number of stages in the cascade

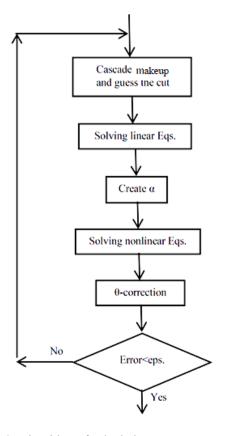


Fig. 3. Algorithm of calculation core

Figure 3 presents the core calculation method. The calculation core in figure 3 has five steps: In the first step, the cascade makeup and the θ are guessed. In the second step, the linear equations are solved. In the third step, the separation factor is created according to enriching and stripping functions. In the fourth step, non-linear equations are solved. In the fifth step, the θ is corrected. In the final step if Error $<\varepsilon$ the calculation core ends else goes to the second step. The error in figure 3 may be the difference between the two iteration parameters.

IV. NUMERICAL RESULTS AND DISCUSSION

The DFUNCAS can design a wide range of cascade kinds. Four test cases were accrued for validation of the proposed design algorithm. The first test case designs a symmetric ideal cascade and the second test case design a symmetric non-ideal cascade. An asymmetric ideal cascade and an asymmetric non-ideal cascade were designed in test cases 3 and 4, respectively.

A. Test Case 1

The general parameters for this test case are given in Table 1. In this test case, the symmetric ideal cascade is designed. Initial data: the separation factors assumed for ideal cascade ($\beta = \gamma = 1.44$), the optimum feed of single machine is 85 gr/hr, the cascade feed 250 gr/hr with natural concentration (0.00711), the concentration of waste and product are 0.003 and 0.03, respectively.

The results are shown in Table 2 and 3. The algorithm designs a 13 stages cascade with 0.0029 and 0.0356 for the concentration of waste and product, respectively. For this design, the non-ideality that is calculated from Eq. (15) is zero.

Table 1General Parameters of Test Case 1

down	up	Optimum feed of single machine gr/hr	Cascade feed gr/hr	X_W	X_P	X_F	α=β*γ
1	1	85	250	0.003	0.03	0.00711	1.44

Table 2 *Results of Test Case 1*

Feed stage	Waste Concentration $x_{\rm w}$	Product Concentration x_p	SWU of Total stage	SWU of cascade	Non-ideality
5	0.0029	0.0356	1296.0848	1296.0848	0

Table 3Detailed Results of Test Case 1

Stage No.	No. Cfg	F	P	W	Xf	Хр	Xw	cut	SWU Stage
Stage 01	5	399.2407	181.5979	217.6427	0.0034	0.0041	0.0029	0.4548	57.9674
Stage 02	9	732.445	33.2043	399.2407	0.0041	0.0049	0.0034	0.4549	106.3468
Stage 03	12	1010.72	459.8727	550.847	0.0049	0.0059	0.0041	0.4550	146.7507
Stage 04	15	1243.341	565.8254	677.5155	0.0059	0.0071	0.0049	0.4551	180.526
Stage 05	17	1438.062	654.5942	783.4681	0.0071	0.0085	0.0059	0.4552	208.7984
Stage 06	13	1142.39	520.1528	622.2369	0.0085	0.0102	0.00711	0.4553	165.8684
Stage 07	11	895.8156	408.0201	487.7956	0.0102	0.0122	0.0085	0.4555	130.0673
Stage 08	8	690.1209	314.4581	375.6628	0.0122	0.0146	0.0102	0.4557	100.2016
Stage 09	6	518.449	236.1008	282.1008	0.0146	0.0175	0.0122	0.4559	75.2758
Stage 10	4	375.0776	171.0867	203.9909	0.0175	0.0209	0.0146	0.4561	54.4591
Stage 11	3	255.2277	116.4983	138.7294	0.0209	0.0251	0.0175	0.4564	37.0576
Stage 12	2	154.9043	70.7633	84.1410	0.0250	0.0299	0.0209	0.4568	22.4912
Stage 13	1	70.7633	32.3573	38.4060	0.0299	0.0356	0.0250	0.4573	10.2744

Table 4Checking the Law of Conservation of Mass and the Law of Conservation of Mass Desired Component for Test Case1

Casei		
Stage No.	F-W-P ×10 ⁻¹²	$F*X_{f}-P*X_{p}-W*X_{w} \times 10^{-12}$
Stage 01	0	0.000888
Stage 02	0	0
Stage 03	0	-0.00089
Stage 04	0	-0.00089
Stage 05	-0.11368	-0.00178
Stage 06	-0.11368	0.00355
Stage 07	0.05684	-0.04263
Stage 08	0	-0.08527
Stage 09	-0.05684	-0.00622
Stage 10	0	-0.06128

Stage No.	F-W-P ×10 ⁻¹²	F*X _f -P*X _p -W*X _w ×10 ⁻¹²
Stage 11	0	0.01332
Stage 12	0	-0.06350
Stage 13	0.00711	0.12834

Checking the law of conservation of mass and the law of conservation of desired mass are given in Table 4. The results show the DFUNCAS has a good performance for designing the symmetric ideal cascade.

B. Test Case 2

The general parameters for this test case are given in Table 5. In this test case, the symmetric non-ideal cascade is designed.

Initial data: the separation factors assumed as functions of feed flow:

$$\beta = 1.74f^{-0.045},\tag{16}$$

$$\gamma = 1.73 f^{-0.05}. \tag{17}$$

The optimum feed of the single machine is 85 gr/hr, the cascade feed is 250 gr/hr with natural concentration (0.00711), and the concentration

of waste and product are 0.003 and 0.03 respectively.

The results are shown in Tables 6 and 7. The algorithm designs a 6 stages cascade with 0.0029 and 0.0321 for the concentration of waste and product, respectively. For this design the non-ideality calculated from Eq. (15) is significant. Figure 4 shows the concentration and flow distribution of in each stage.

Table 5 *General Parameters of Test Case 2*

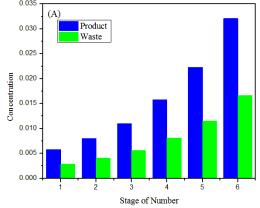
down	up	Optimum feed of single machine gr/hr	Cascade feed gr/hr	X_W	X_P	X_F	γ	β
1	1	85	250	0.003	0.03	0.00711	1.73*f^(-0.05)	1.74*f^(-0.045)

Table 6
General Results of Test Case 2

Feed stage	Waste Concentration x_w	Product Concentration x_p	SWU of Total stage	SWU of cascade	Non-ideality
3	0.0029	0.0321	1215.3059	1202.1999	0.0109

Table 7Detailed Results of Test Case 2

Stage No.	No. Cfg	F	P	W	Xf	Хр	Xw	cut	SWU Stage
Stage 01	4	355.1611	140.8948	214.2663	0.0041	0.0058	0.0029	0.3967	174.4986
Stage 02	7	588.6519	233.4907	355.1611	0.0056	0.0080	0.0041	0.3966	294.4301
Stage 03	9	742.4814	294.7243	447.7571	0.0077	0.0110	0.0056	0.3969	372.6915
Stage 04	5	429.9852	170.9946	258.9906	0.0112	0.0158	0.0081	0.3977	213.9597
Stage 05	3	224.6553	89.3944	135.2609	0.0160	0.0223	0.0115	0.3979	115.5349
Stage 06	1	89.3944	35.7337	53.6607	0.0227	0.0321	0.0166	0.3997	44.1912



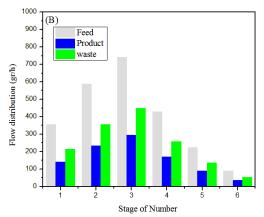


Fig. 4 (A) The Concentration and (B) Flow Distribution of in Each Stag

Checking the law of conservation of mass and the law of conservation of desired mass are given in Table 8. Table 8 shows that the DFUNCAS has a good performance for designing the symmetric non-ideal cascade.

C. Test Case 3

The general parameters for this test case are given in Table 9. In this test case the asymmetric ideal cascade is design. Initial data: the stage configuration is 2-up 1-down, the separation factors assumed for ideal cascade ($\gamma = \beta^2 = 2.56$), the optimum feed of single machine is 85 gr/hr, the cascade feed 250 gr/hr with natural concentration (0.00711), the concentration of waste and product are 0.003 and 0.03, respectively.

The results are shown in Table 10 and 11. The algorithm designs a 5 stages cascade with 0.0017 and 0.0448 for concentration of waste and product respectively. For this design the non-ideality that calculated from Eq. (15) is zero.

Table 8Checking the Law of Conservation of Mass and the Law of Conservation of Mass Desired Component for Test Case 2

<i>F-W-P</i> ×10 ⁻¹³	$F*X_{f}-P*X_{p}-W*X_{w} \times 10^{-14}$
0	0
0.2842	0.0444
0	0
0.2842	0
-0.1421	-0.1776
-0.0711	0.2220
	×10 ⁻¹³ 0 0.2842 0 0.2842 -0.1421

Table 9

General Parameters of Test Case 3

down	up	Optimum feed of single machine gr/hr	Cascade feed gr/hr	X_W	X_P	X_F	γ	β
2	1	85	250	0.003	0.03	0.00711	2.56	1.6

Table 10 *Results of Test Case 3*

Feed stage	Waste Concentration x_w	Product Concentration x_p	SWU of Total stage	SWU of cascade	Non-ideality
2	0.0017	0.0448	1626.9440	1626.9439	0

Table 11Detailed Results of Test Case 3

Stage No.	No. Cfg	F	P	W	Xf	Хр	Xw	cut	SWU Stage
Stage 01	1	100.1695	50.5575	49.612	0.0046	0.0071	0.0017	0.5047	201.3756
Stage 02	4	351.1654	177.6988	173.4667	0.0071	0.0113	0.0028	0.5060	705.3855
Stage 03	2	203.3077	103.1382	100.1695	0.0113	0.0180	0.0044	0.5073	408.1375
Stage 04	1	103.1382	52.5302	50.6079	0.0180	0.0285	0.0071	0.5093	206.8508
Stage 05	1	52.5302	26.9213	25.6089	0.0285	0.0448	0.0113	0.5125	105.1947

Checking the law of conservation of mass and the law of conservation of desired mass are given in Table 12. The results show the DFUNCAS has a good performance for designing the asymmetric ideal cascade.

D. Test Case 4

The general parameters for this test case are given in Table 13. In this test case, the symmetric non-ideal cascade is designed. Initial data: the separation factors assumed as functions of feed flow:

$$\beta = 2.7f^{-0.045},\tag{18}$$

$$\gamma = 1.65 f^{-0.05}. \tag{19}$$

The optimum feed of the single machine is 85 gr/hr, the cascade feed is 250 gr/hr with natural concentration (0.00711), and the

concentration of waste and product are 0.003 and 0.03 respectively.

The results are shown in Tables 14 and 15. The algorithm designs a 6 stages cascade with 0.003 and 0.0416 for the concentration of waste and product respectively. For this design the non-ideality that was calculated from Eq. (15) is significant.

Table 12Checking the Law of Conservation of Mass and the Law of Conservation of Mass Desired Component for Test Case3

Stage No.	<i>F-W-P</i> ×10 ⁻¹³	$F*X_{f}-P*X_{p}-W*X_{w} \times 10^{-14}$
Stage 01	0	0.0111
Stage 02	0	-0.0888
Stage 03	0	0.0444
Stage 04	0	0.1332
Stage 05	0	-0.4663

Table 13General Parameters of Test Case 4

down	up	Optimum feed of single machine gr/hr	Cascade feed gr/hr	Xw	X_P	X_F	γ	β
1	2	85	250	0.003	0.03	0.00711	1.65*f^(-0.05)	2.7*f^(-0.045)

Table 14Results of Test Case 4.

Feed stage	Waste Concentration x_w	Product Concentration x _p	SWU of Total stage	SWU of cascade	Non-ideality
4	0.003	0.0416	1343.4734	1233.1283	0.0895

Table 15Detailed Results of Test Case 4

Detailed Resi	iiis oj 1 esi	cuse i							
Stage No.	No. Cfg	F	Р	W	Xf	Хр	Xw	cut	SWU Stage
Stage 01	3	262.0139	43.9784	218.0354	0.0039	0.0087	0.003	0.1678	227.0911
Stage 02	4	315.3044	53.2906	262.0139	0.0052	0.0115	0.0039	0.1690	279.0026
Stage 03	4	378.7596	63.4552	315.3044	0.0068	0.0149	0.0052	0.1675	321.9865
Stage 04	5	403.1431	68.3619	334.7812	0.0087	0.0191	0.0066	0.1696	355.6696
Stage 05	1	119.7933	19.9408	99.8525	0.0147	0.0314	0.0113	0.1664	96.4876
Stage 06	1	68.3619	12.0237	56.3381	0.0191	0.0416	0.0143	0.1759	63.2301
Stage 06	1	68.3619	12.0237	56.3381	0.0191	0.0416	0.0143	0.17	59

Checking the law of conservation of mass and the law of conservation of desired mass are given in Table 16. Table 16 shows that the DFUNCAS has a good convergence for designing the asymmetric non-ideal cascade.

In test case 3, the values of β and γ were constant and the non-ideality value was zero, while in test case 4, the values of β and γ were variable (feed flow) and the non-ideality value was close to zero, so the difference in test case results in 4 and 3 is significant.

V. CONCLUSION

This theory for the separation of binary mixtures based on a single machine functional equation has been developed. The dependence of separation factors on feed has been used to simulation the symmetrical or unsymmetrical cascade. Design the functional cascades (DFUNCAS) has been introduced to design the cascade. The relationship between the separation factor and feed is determined from the results of these calculations. In the future, we plan to optimize the cascade simulation. The results showed the DFUNCAS has a good performance for simulating the symmetrical or unsymmetrical cascade. This simulation will allow decreasing expenses.

Table 16Checking the Law of Conservation of Mass and the Law of Conservation of Mass Desired Component for Test Case4

Stage No.	F-W-P ×10 ⁻¹³	F*X _f -P*X _p -W*X _w ×10 ⁻¹⁵
Stage 01	0.0710	-0.2220
Stage 02	-0.0710	-0.2220
Stage 03	-0.28422	0
Stage 04	0.1421	0
Stage 05	0.0710	0.2220

REFERENCES

- 1. R.V. Wissen, M. Golombok, J.J.H. Brouwers, Separation of carbon dioxide and methane in continuous countercurrent gas centrifuges. Chem. Eng. Sci. 60, 4397-4407 (2005).
- 2. M. Khajenoori, et al, Investigation of hydrodynamic parameters inside a gas centrifuge rotor in the presence of hydrogen fluoride and air light gases using DSMC and Boltzmann distribution function.

 Journal of Nuclear Science and Technology, 94(4), 1-6 (2021).
- M. Khajenoori, et al, Modeling and simulating of feed flow in a gas centrifuge using the Monte Carlo method to calculate the maximum separation power. Journal of Molecular Modeling 25(11), 1-12 (2019). https://doi.org/10.1007/s00894-019-4226-x
- 4. M. Khajenoori, et al. Modeling gas-granular flow in molecular using the DSMC method and continuum regions by Onsager's pancake equation with mass sources and sinks in a rotating cylinder. Granular Matter 21(3), 1-15 (2019). https://doi.org/10.1007/s10035-019-0920-8
- 5. S. Yousefi-Nasab, et al, *Prediction of the compression ratio of a Holweck-type molecular pump with the presence of multi-component gases using a modified Sickafus method for high-speed rotors.* Vacuum, 172, 109056 (2020). https://doi.org/10.1016/j.vacuum.2019.109056
- 6. J. Safdari, A. Norouzi, R. Tumari, *Using a real coded PSO algorithm in the design of a multi-component countercurrent cascade.* Separation Science and Technology, 52(18), 2855-2862 (2017).
- 7. G. Geldenhuys, *Design of an Asymmetric Ideal Cascade for Isotope Enrichment*. SIAM Review. 21, 390-394 (1979).
- 8. H.G. Wood, et al, Estimation of overall separation factor of a gas centrifuge for different multicomponent mixtures by separation theory for binary case. Sep. Sci. and Tech. 37, 417-430 (2002).

- 9. F. Deneddu, P. Robin, H.G. Wood, *Optimization studies for Gas Centrifuges*. Sep. Sci. and Tech. 35, 1207-1221 (2000).
- J. Hu, C. Ying, S. Zeng, Overall separation factor in a gas centrifuge using a purely axial flow model. Sep. Sci. and Tech. 40, 2139-2152 (2005).
- 11. V.A. Palkin, Determination of the optimal parameters of a cascade of gas centrifuges.

 Atomic Energy. 84, 190–195 (1998).
- A. Norouzi, A.H. Minuchehr, A. Zolfaghari, A. Hagighattalab, Parameters Optimization of a Counter-Current Cascade Based on Using a Real Coded Genetic Algorithm. Sep. Sci. and Tech. 46, 2223-2230 (2011). https://doi.org/10.1080/01496395.2011.595473
- 13. V.A. Palkin, I.S. Igoshin, Determination of the Optimal Parameters of a Gas Centrifuge Cascade with an Arbitrary Stage Connection Scheme. Atomic Energy. 112, 47–52 (2012).
- 14. V. Borisevich, M. Borshchevskiy, S. Zeng, D. Liang, On ideal and optimum cascades of gas centrifuges with variable overall separation factors. Chem. Eng. Sci. 116, 465-472 (2014).
- 15. A.Y. Smirnov, G.A. Sulaberidze, Q. Xieb, V.D. Borisevich, *Design of cascade with locally enlarged flow for enrichment of intermediate components of multi-isotope mixtures*. Chem. Eng. Res. Des. 95, 47–54 (2015).