M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

An Optimized Search Algorithm for Charged Fuel Enrichment in Fixed-Source Equilibrium Cycle Analysis of REBUS-3

Tongkyu Park[a,b] and Won Sik Yang[a]

a) School of Nuclear Engineering, Purdue University, 400 Central Dr., West Lafayette, IN 47907, USA
b) FNC Technology, Heungdeok IT Valley Bldg. 32F, 13, Heungdeok 1-ro, Yongin-si, Gyeonggi-do, 446-908, Korea
park723@purdue.edu; yang494@purdue.edu

Abstract – *This paper presents an optimized search algorithm for the charged fuel enrichment in fixed-source equilibrium cycle analysis of REBUS-3. The charged fuel enrichment search for a fixed-source equilibrium cycle problem is performed in two steps. The enrichment search is first done for the corresponding eigenvalue problem to determine the nuclide densities of burned fuels approximately, and then the enrichment for the fixed source problem is determined to meet the imposed constraints. A new enrichment search algorithm has recently been developed to minimize the required number of flux calculations for eigenvalue problems. This algorithm has been further optimized for fixed-source problems using a partially converged solution of the corresponding eigenvalue problem. To verify the effectiveness and efficiency of the optimized algorithm, a series of sensitivity analyses have been performed using an accelerator driven system and a wide range of user-specified initial guesses. Numerical results showed that the optimized search algorithm could reduce the number of flux calculations by a factor of 1.6 and 1.2, respectively, compared to the original and the recently developed search algorithms. Furthermore, the results showed that the performance of the optimized search algorithm is insensitive to the user-specified enrichment parameter guesses as well.*

I. INTRODUCTION

The REBUS-3 code [1,2] is a system of programs designed for the fuel cycle analysis of fast reactors. It can analyze the non-equilibrium cycle as well as the equilibrium cycle of fast reactors. To reduce the manual iterations of core designs, the existing REBUS-3 code provides four search capabilities to determine various design parameters so that desired values of performance parameters can be achieved [1-3]. Among those, the most useful and commonly used capability for core design studies is the search of the charged fuel enrichment to achieve a specified value at a specified time during the burn cycle of the k-effective (k-eff) for eigenvalue problems or the source multiplication factor (k-src) for fixed-source problems.

However, the convergence rate of the charged fuel enrichment search highly depends on the two user-specified initial guesses. If the user-specified guesses are close to the final enrichment to yield the targeted k-eff or k-src value of the problem, a converged solution can be obtained relatively quickly. Otherwise, it takes a large number of iterations (i.e., fuel cycle calculations) to yield a converged solution or even terminates the job with no converged solution. In general, the user cannot make good guesses for the enrichment beforehand and therefore it is desirable to develop an enrichment search algorithm that is less sensitive to the user-specified enrichment guesses.

To resolve this convergence problem of the existing search algorithm in REBUS-3, a new search algorithm for the charged fuel enrichment has recently been developed for the equilibrium cycle analysis of REBUS-3 [4]. The new search algorithm (hereafter, enhanced search algorithm) is based on the idea of reducing the number of enrichment estimates by allowing drastic enrichment changes and by optimizing the acceleration scheme of the original search algorithm. Test results showed that the enhanced search algorithm is able to produce a converged solution regardless of the initial guess. In addition, it reduced the number of flux calculations by a factor of 2.9 and 1.8 for eigenvalue problems with recycling and without recycling, respectively, compared to the existing search algorithm [4].

In this work, the enhanced search algorithm was further optimized for fixed-source equilibrium cycle problems. In a fixed-source equilibrium cycle problem, the enrichment estimates should remain within the subcritical range. Otherwise, the flux calculation would diverge. Since the subcritical enrichment range for a given source distribution is not readily available, initial values for the charged fuel enrichment and the nuclide densities of burned fuels are prepared by solving the corresponding eigenvalue problem with no source [2]. As a result, for a fixed-source equilibrium cycle problem, two enrichment search calculations are sequentially performed: one for the eigenvalue problem and the other for the fixed-source problem.

In the new optimized search algorithm, the number of fuel cycle calculations is minimized by a partial convergence of the enrichment search for the eigenvalue problem and thus the number of flux calculations and the computational time are further reduced compared to the counterparts obtained from the enhanced search algorithm. The effectiveness and efficiency of the optimized algorithm for fixed-source equilibrium cycle problems were examined using a series of sensitivity analyses with an 840 MWt accelerator driven system (ADS) and a wide range of initial guesses.

II. CHARGED FUEL ENRICHMENT SEARCH ALGORITHMS

In REBUS-3, multiple fuel types are allowed and represented by a material type l and different burned stages of each fuel is represented by a stage number τ, which is the number of burn cycles plus one. Denoting the τ-th stage density vector of the l-th material as $\mathbf{n}_{l,\tau}(t)$ and assuming a total of L material types are loaded into the core and the l-th material successively resides in the core during $S(l)$ cycles until it is discharged, the nuclide density vector of all fuels at time t can be defined as

$$\tilde{\mathbf{n}}_m(t)=\left[\mathbf{n}_{1,1}(t),\mathbf{n}_{1,2}(t),\cdots,\mathbf{n}_{1,S(1)}(t),\cdots,\mathbf{n}_{L,S(L)}(t)\right]^T. \quad (1)$$

With this notation, the nuclide density vectors of charged and discharged fuels can be written as in Eq. (2) and Eq. (3), respectively,

$$\tilde{\mathbf{n}}_c=\left[\mathbf{n}_{1,1}(0),\mathbf{n}_{2,1}(0),\cdots,\mathbf{n}_{L,1}(0)\right]^T, \quad (2)$$

$$\tilde{\mathbf{n}}_d=\left[\mathbf{n}_{1,S(1)}(T),\mathbf{n}_{2,S(2)}(T),\cdots,\mathbf{n}_{L,S(L)}(T)\right]^T, \quad (3)$$

where T is the cycle length.

At the beginning of calculation, the charged fuel density vector $\tilde{\mathbf{n}}_c^{(0)}$ is determined using the user-specified enrichment guess and external feed density vector $\tilde{\mathbf{n}}_f$, as schematically shown in Fig. 1. In REBUS-3, the enrichment of a charged fuel is defined as a volume ratio of Class 1 fuel to Class 1 and Class 2 fuels. The Class 1 fuel is the feed stream of high reactivity fuel and the Class 2 fuel is the feed stream of low reactivity fuel [1,3]. The enrichment e of a charged fuel is determined as,

$$e=e_0[1+(x-1.0)\delta] \quad (4)$$

where e_0 and δ are the user-specified initial enrichment and enrichment modification factor, respectively. The variable x is the charged fuel enrichment parameter to be determined iteratively in the search procedure, and its two initial guesses, $x^{(0)}$ and $x^{(1)}$, are specified by the user. Since the resulting enrichment e should be between 0 and 1, for given e_0 and δ, x should be in the range between the lower bound $x_L=1-1/\delta$ and the upper bound $x_U=1+(1/e_0-1)/\delta$.

For a given enrichment parameter, the stage density vectors are determined through the cyclic mode iteration scheme as shown in Fig. 2. At the beginning of the cyclic mode calculation, the charged fuel density is used as the initial guess for all the stage densities. With the known nuclide density vectors at the beginning of cycle, the stage densities are determined by depleting the charged fuel vector using the neutron fluxes determined by solving the coupled neutron transport and nuclide depletion equations iteratively.

For the neutron transport calculation, the nuclide density vector in a spatial region k is computed as

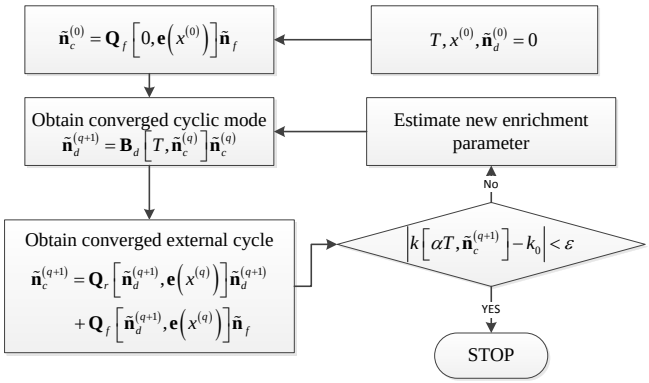

Fig. 1. Charged fuel enrichment search algorithm of REBUS-3.

$$\mathbf{n}_k(t)=\frac{1}{V_k}\sum_{l,\tau\in V_k}\mathbf{n}_{l,\tau}(t)V_l \quad (5)$$

where V_k is the volume of region k and V_l is the volume of material type l in region k. For a given stage density vectors at the beginning of time step, the stage density vectors at the end of time step are determined by solving the depletion equation with the average of the beginning and the end of cycle fluxes. That is, the $(\tau+1)$-st stage density vectors are sequentially computed as

$$\mathbf{n}_{l,\tau}(0)=\left\{\prod_{j=1}^{\tau-1}\mathbf{B}_{l,j}\left[T,\tilde{\mathbf{n}}_m(0)\right]\right\}\mathbf{n}_{l,1}(0) \quad (6)$$

where $\mathbf{B}_{l,j}$ is the exponential of burn matrix for the fuel of material type l and stage number j. Since the neutron flux and the region density vector at the end of time step are coupled, they are solved iteratively using the region density iteration scheme [3].

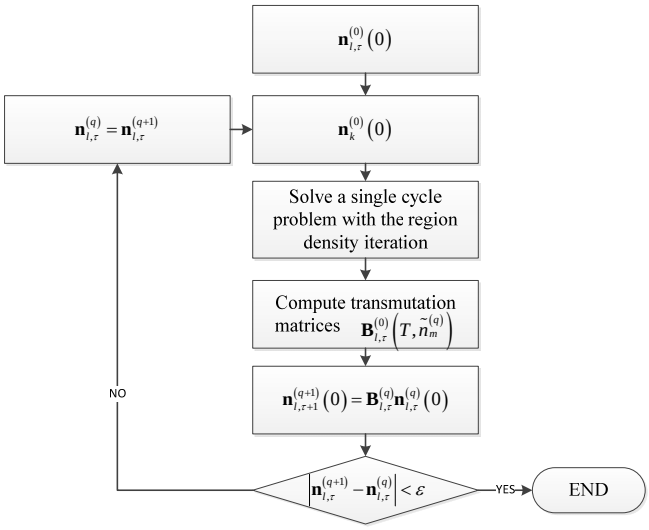

Fig. 2. Cyclic mode iteration scheme of REBUS-3

The discharge density vector $\tilde{\mathbf{n}}_d^{(q+1)}$ for the $(q+1)$ -st charged fuel enrichment iteration step can be determined by the cycle length T and the q -th charged density vector as

$$\tilde{\mathbf{n}}_d^{(q+1)} = \mathbf{B}_d \left[T, \tilde{\mathbf{n}}_c^{(q)} \right] \tilde{\mathbf{n}}_c^{(q)} \tag{7}$$

where $\mathbf{B}_d$ is the exponential of burn matrix for discharge. With $\tilde{\mathbf{n}}_d^{(q+1)}$ calculated from the cyclic mode iteration, the charged density vector $\tilde{\mathbf{n}}_c^{(q+1)}$ at the $(q+1)$ -st iteration step is updated in the external cycle iteration as

$$\tilde{\mathbf{n}}_c^{(q+1)} = \mathbf{Q}_r \tilde{\mathbf{n}}_d^{(q+1)} + \mathbf{Q}_f \tilde{\mathbf{n}}_f \tag{8}$$

where $\mathbf{Q}_r$ is the delivery matrix for the reprocessing process and $\mathbf{Q}_f$ is the delivery matrix for the external feed. The two delivery matrices $\mathbf{Q}_r$ and $\mathbf{Q}_f$ are iteratively computed in the external cycle iteration. The charged density vector is determined to satisfy the isotopic mass balances during the external cycle operations such as reprocessing of discharged fuel, refabrication of charged fuel, etc. Note that the delivery matrices depend on the discharge density vector $\tilde{\mathbf{n}}_d$ and the charged fuel enrichment e.

Once the stage density and external cycle iterations have converged, the equilibrium cycle analysis for a given enrichment parameter is completed. Thus, the k-eff or k-src value at a user-specified fraction α of the cycle length T is obtained. If this value is close to the user-specified target value k_0 within the user-specified convergence criterion ε, the search procedure is terminated. Otherwise, REUBS-3 estimates a new enrichment parameter x and repeats the equilibrium cycle analysis. Starting from two user-specified initial guesses, a new estimate of the enrichment parameter is determined by interpolating the latest two or three enrichment parameters and the corresponding k-eff or k-src values.

Since the original and enhanced search algorithms for the charged fuel enrichment are described in detail elsewhere [3,4], their main properties are briefly presented below. Then the primary characteristics of the optimized search algorithm for fixed-source problems are discussed.

1. Original Search Algorithm

In the original search algorithm for the charged fuel enrichment, a new estimate for the charged fuel enrichment is determined by a linear or quadratic interpolation of the latest two or three data points of the enrichment parameter and the corresponding k-eff or k-src values. One of the conditions imposed in the original algorithm is that it does not allow a drastic change in enrichment parameter. It limits the maximum allowable change to the 10 percent of the preceding enrichment parameter. If an estimated enrichment is smaller than x_L, the enrichment search is abnormally terminated.

The charged fuel enrichment search algorithm shown in Fig. 1 requires a substantial amount of computational time since each iteration for estimating a new enrichment parameter involves a complete analysis of the equilibrium cycle corresponding to the estimated enrichment parameter. To reduce the computational time, REBUS-3 has three different levels of search procedures: preliminary, intermediate, and final search levels. The three levels of search procedures are invoked sequentially to determine the charged fuel enrichment that yields the equilibrium cycle solution with the targeted performance parameters. The preliminary and intermediate search levels are simple variations of the final search level with reduced numbers of permissible iterations of cyclic mode and region densities.

At the preliminary search level, the cyclic equilibrium solution is approximately obtained with two region density iterations, one cyclic mode iteration, and no external cycle iteration. The whole cycle length is represented as a single time interval, regardless of the user-specified number of subintervals. In addition, for high burnup problems, the convergence criterion of k-eff or k-src to a targeted value is temporarily increased by a factor of 50 [3,4].

If the enrichment parameter converges at the preliminary search level, the intermediate search is initiated with refined computational models to obtain a better enrichment estimate. Specifically, the time domain is divided into the user-specified number of subintervals and full external cycle iterations are made. However, the region density and cyclic mode iterations are limited to one. If the enrichment parameter converges at the intermediate search level again, then the final search level is invoked with full iterations for region density, cyclic mode, and external cycle calculations.

2. Enhanced Search Algorithm

In the enhanced search algorithm, drastic changes in the enrichment are allowed, and a new estimate is determined by the linear interpolation of the latest two values for all the equilibrium cycle problems. If the first estimate computed with the two user-specified initial guesses is non-physical (i.e., either smaller than x_L or greater than x_U), the initial user-specified enrichment parameter is reused as the third enrichment parameter instead of the first computed estimate.

If a non-physical enrichment parameter is encountered again in the subsequent iteration process, the non-physical estimate is reset according to the following rules. If the new estimate is smaller than x_L, it is set to 90% of the smaller value of the latest two enrichment parameters. If the estimate is greater than x_U, it is set to 110% of the larger one of the latest two values.

In addition, the intermediate search level is removed and full external cycle iterations are carried out at the preliminary search level. The rule for temporarily increased convergence criterion for high discharge burnup problems is also removed.

3. Optimized Search Algorithm for Fixed-Source Problem

For a given charged fuel enrichment, the k-src of the fixed-source problem and the k-eff value of the corresponding eigenvalue problem are different. Therefore, the enrichment search for the fixed-source problem should be carried out even when the eigenvalue problem yields the targeted k-eff value. This suggests that for a fixed-source problem, a tight convergence of charged fuel enrichment might not be necessary in the corresponding eigenvalue problem. Based on this observation and the results of parametric studies, new rules were developed for the enrichment search in the corresponding eigenvalue problem.

The convergence criterion of k-eff is increased by a factor of 10 relative to that of k-src. Since they are calculated with not fully converged stage and region densities, the k-eff values of the first few iterations of the preliminary search might be quite different from the values calculated with the fully converged stage and region densities. As a result, the preliminary search procedure might generate a speciously converged solution. To avoid a false convergence, the last estimate of the preliminary search is reanalyzed in the final search with reduced numbers of permissible iterations of stage and region densities as the preliminary search.

In addition, the new rules to reset a non-physical enrichment parameter were slightly changed. If a new estimate is smaller than x_L, it is set to 10% of the smaller value of the latest two enrichment parameters.

III. NUMERICAL RESULTS

To verify the effectiveness and efficiency of the optimized enrichment search algorithm compared to the original and enhanced enrichment search algorithms, a series of sensitivity analyses were performed for the fixed-source equilibrium cycle problem of an 840 MWt ADS and 50 randomly generated initial and second enrichment parameters.

1. Description of a Test Problem

A design of an 840 MWt sodium-cooled ADS blanket with a zirconium-matrix minor actinide (MA) dispersion fuel [5,6] was used to investigate the efficiency of the optimized search algorithm for the charged fuel enrichment in fixed-source equilibrium cycle problems.

The ADS blanket layout is illustrated in Fig. 3. The system is composed of 19 hexagonal assembly positions for the lead bismuth eutectic (LBE) target and buffer, 132 fuel assemblies, 102 steel reflectors, and 60 B_4C radial shields. The 132 fuel assemblies are divided into three zones of different fuel-particle volume fractions (i.e., inner, middle and outer zones) to flatten the power distribution. The ADS blanket burns the MA recovered from the sodium-cooled fast reactor with MA target assemblies [7]. The discharged fuel of ADS is reprocessed and all the recovered heavy metal is recycled into ADS. The fuel management scheme and the fuel residence time were determined to satisfy the peak fast fluence limit. Each fuel assembly remained in the same position without shuffling or rotation until it was discharged. Higher fast flux occurs in the inner zone because the spallation neutron source is concentrated in the target. In order to meet the peak fast fluence limit, the fuel residence time was reduced for the inner zone. A six-month cycle length with a capacity factor of 75% was used with 7-batch fuel management scheme for the inner zone and an 8-batch scheme for the middle and outer zones.

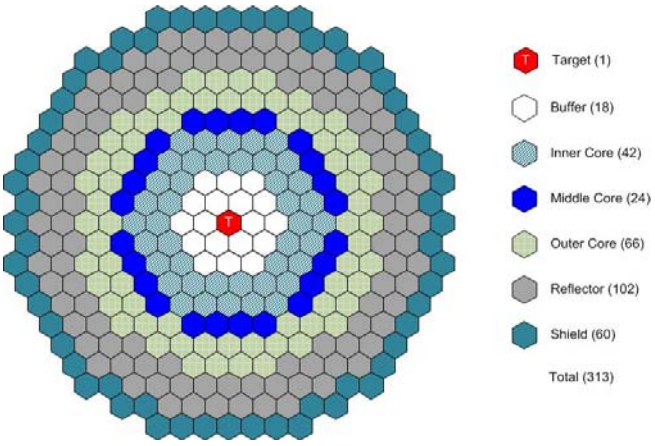

Fig. 3. Radial core layout of 840 MWt ADS blanket.

The equilibrium cycle of ADS blanket was analyzed by using the ANL suite of fast reactor analysis codes. An inhomogeneous fixed-source problem was solved for the blanket with the triangular-z finite difference option of the DIF3D code [8,9], using a generic distribution of spallation neutron source generated for a 1 GeV proton beam and a prototypic LBE target [10]. Then, depletion calculations were performed at a constant power level by increasing the source intensity over an operating cycle to compensate for the burnup reactivity loss. Region-dependent cross sections were generated in a 33-group energy structure using the MC^2-3 code [11] and the ENDF/B-VII.0 data. The scattered loading approximation [1] is used for reflecting the given fuel management schemes. In this scattered loading approximation, approximate batch-averaged equilibrium cycle is considered and it is assumed that all stages of fuel have equal volume fractions in the fuel assembly.

The fraction of MA-10Zr fuel particles in fuel was determined to attain a k-src value of 0.97 at the beginning of equilibrium cycle (BOEC). The maximum allowable relative error in any isotope region density was 0.001. The maximum allowable relative errors in stage and charge fuel densities were set to 0.001 and 0.0001, respectively. The convergence criterion for k-src was set to 0.0001. δ in Eq. (4) is specified as 1 for all the batch types and thus the lower bound x_L is 0.

2. Sensitivity Analyses

Fifty enrichment search cases were defined for the equilibrium cycle of ADS with randomly generated user-specified enrichment parameters. High discharge burnup option was specified for the original search algorithm because the average discharge burnup of this ADS blanket was approximately 27.8%. Since the only difference among those 50 cases is the two user-specified enrichment parameters, it is expected that the final solution of the 50 cases should be practically the same. It is obvious that the difference in k-src will be less than 20 pcm when a converged solution is obtained because the relative error allowable in k-src during enrichment search procedure was set to 0.0001. The converged enrichment parameter x_c for this problem is 0.153 and the converged fuel enrichment is 11.4%.

Table I shows the total number of flux calculations required to obtain the final converged solution for a given pair of user-specified enrichment parameters. The original REBUS-3 code produced the converged solutions for 16 cases only. For the remaining 34 cases, the search process was abnormally terminated because a negative enrichment estimate (i.e., enrichment parameter x smaller than x_L) was encountered. On the other hand, the enhanced and optimized algorithms were able to produce a final converged solution regardless of user-specified parameters. Furthermore, they improve the computational efficiency for all the 50 cases considered. The enhanced and optimized search algorithms significantly reduce the total number of flux calculations required to yield the final converged solution. The original algorithm requires 98.4 flux calculations on average for the 16 converged cases. For these cases, relative to the original search algorithm of REBUS-3, the enhanced and optimized algorithms reduce the number of flux calculations by a factor of 1.4 and 1.6, respectively. The average number of flux calculations for all the 50 cases is 77.2 for the enhanced algorithm and 65.9 for the optimized algorithm.

Table II shows the list of the best enrichment parameter guesses for the 16 converged cases among a total of 50 cases compared to the converged solution of 0.153. The ranking in the fourth column is considered with the initial enrichment parameter guess while that in the fifth column is obtained with only the second enrichment parameter guess. The ranking obtained with both of the initial and second enrichment parameter guesses is listed in the last column. Compared to the converged solution of 0.153, it can be seen that the best initial guesses were given in the order of Case 41, 39, 7, 30, 1, and 10 according to the ranking in the last column. On the other hand, Cases 21, 40, 32, 6, and 27 are the five worst cases among the 50 cases.

Even though a relatively good initial guesses was provided for Case 10 (i.e., 6th best guess), the original algorithm was not able to produce a converged solution. Note that the ranking of Case 10 is 2 and 18 for the first two

Table I. Randomly Selected 50 Pairs of Enrichment Parameter Guesses and the Numbers of Flux Calculations of Original, Enhanced and Optimized Search Algorithms

Case No.	Enrichment parameter guesses		Number of flux calculations		
	initial	second	original	enhanced	optimized
1	0.250	0.163	104	54	48
2	0.688	0.537	-	66	62
3	0.767	0.313	-	71	65
4	0.576	0.279	122	65	57
5	0.338	0.119	79	63	59
6	0.875	0.725	-	63	59
7	0.220	0.181	119	57	53
8	0.363	0.049	112	74	58
9	0.843	0.285	-	66	65
10	0.168	0.026	-	74	66
11	0.470	0.604	-	80	69
12	0.524	0.691	-	80	72
13	0.675	0.879	-	99	76
14	0.001	0.029	130	78	71
15	0.413	0.882	-	87	86
16	0.848	0.555	-	78	73
17	0.551	0.467	-	63	63
18	0.711	0.594	-	63	59
19	0.489	0.359	-	65	59
20	0.109	0.451	-	63	59
21	0.975	0.982	-	122	68
22	0.742	0.697	-	92	69
23	0.007	0.075	100	84	86
24	0.974	0.040	-	81	75
25	0.028	0.997	-	98	81
26	0.782	0.732	-	111	69
27	0.893	0.664	-	71	58
28	0.672	0.769	-	99	73
29	0.547	0.913	-	93	73
30	0.196	0.214	92	60	45
31	0.496	0.190	108	60	59
32	0.766	0.895	-	111	77
33	0.740	0.427	-	78	73
34	0.027	0.110	90	75	69
35	0.157	0.612	-	66	66
36	0.023	0.901	-	99	84
37	0.814	0.110	88	63	55
38	0.941	0.254	86	71	57
39	0.192	0.104	82	65	59
40	0.748	0.954	-	102	69
41	0.099	0.181	90	65	59
42	0.394	0.579	-	80	74
43	0.640	0.901	-	110	81
44	0.801	0.664	-	63	63
45	0.022	0.082	94	81	72
46	0.403	0.125	79	72	58
47	0.927	0.372	-	74	63
48	0.307	0.458	-	72	66
49	0.176	0.452	-	71	59
50	0.452	0.373	-	63	55
average			98.4	77.2	65.9

methods listed in Table II, respectively. The average number of flux calculations for the 10 best cases is 68.4 for the enhanced algorithm and 61.0 for optimized algorithm. For the 10 worst cases, the enhanced and optimized algorithms require 94.5 and 69.3 flux calculations, respectively. The optimized algorithm shows a much smaller variation in the number of flux calculations than the enhanced algorithm. This indicates that the optimized algorithm is less sensitive to the initial guesses than the enhanced algorithm. In addition, the optimized algorithm is more effective than the enhanced algorithm except for Case 23. Averaged over all the 50 cases considered, the optimized search algorithm improves the computational efficiency by 17% relative to the enhanced search algorithm.

Table II. List of Best Enrichment Parameter Guesses with Three Different Methods for the 16 Converged Cases among a Total of 50 Cases

Case No.	Enrichment parameter guesses		Ranking with		
	initial	second	$\left\|x^{(0)}-x_c\right\|$	$\left\|x^{(1)}-x_c\right\|$	Sum[a]
1	0.250	0.163	9	1	5
4	0.576	0.279	29	17	21
5	0.338	0.119	17	5	9
7	0.220	0.181	8	2	3
8	0.363	0.049	18	14	13
14	0.001	0.029	15	16	11
23	0.007	0.075	14	12	10
30	0.196	0.214	5	10	4
31	0.496	0.190	25	6	16
34	0.027	0.110	11	7	7
37	0.814	0.110	42	8	23
38	0.941	0.254	48	13	30
39	0.192	0.104	4	9	2
41	0.099	0.181	7	3	1
45	0.022	0.082	13	11	8
46	0.403	0.125	20	4	12

a) $\left|x^{(0)}-x_c\right|+\left|x^{(1)}-x_c\right|$

Table II also shows that the second enrichment parameter guess is more important than the initial enrichment parameter guess of the original search algorithm for this fixed-source problem. It means even though good initial enrichment parameter is initially specified, the original search algorithm cannot use it effectively because the number of permissible cyclic mode and region density iterations is limited. On the other hand, since the stage densities corresponding to the initial guess are used as the initial values for the stage densities for the second guess, the fuel cycle calculation corresponding to the second guess can be performed more accurately compared to that corresponding to the initial guess.

Table III compares the number of fuel cycle calculations in the initial eigenvalue problem and the actual fixed-source problem and the overall computational time between the original and optimized search algorithms for the 16 converged cases of the original search algorithm. Except for Case 23, the optimized search algorithm reduces the number of fuel cycle calculations (i.e., the number of enrichment estimates) in the initial eigenvalue problem relative to the original search algorithm of REBUS-3. Even in the Case 23 for which the optimized search algorithm requires one more enrichment estimate than the original search algorithm, the total computational time is reduced by 11% because of the reduced number of flux calculations due to the loosened convergence of k-eff in the first-stage eigenvalue problem in the optimized search algorithm. The results in Table III show that the optimized search algorithm can reduce the computational time by a factor of 1.5 on average compared to the original search algorithm. Relative to the original search algorithm, the optimized search algorithm reduces the number of fuel cycle calculations by a factor of 1.8 in the first-stage eigenvalue problem and by a factor of 1.1 in the fixed-source problem.

Table III. Numbers of Equilibrium Cycle Calculations in the Eigenvalue and Fixed-Source Problems and Computational Time for the 16 Converged Cases of Original Search Algorithm

Case No.	Search algorithm					
	Original			Optimized		
	Number of fuel cycle calculations		Time, sec	Number of fuel cycle calculations		Time, sec
	k-eff	Source		k-eff	Source	
1	20	7	268	6	6	149
4	25	7	306	9	6	167
5	10	7	225	9	7	176
7	24	8	303	7	7	162
8	21	7	278	9	6	173
14	26	7	316	13	7	203
23	16	7	265	17	7	235
30	13	8	260	5	6	147
31	21	6	284	9	7	175
34	13	7	239	13	6	190
37	12	7	242	8	6	167
38	11	7	255	9	6	169
39	11	7	227	9	7	176
41	11	7	245	9	7	176
45	15	7	248	14	6	199
46	10	7	224	9	6	166
Avg.	16.2	7.1	261.6	9.7	6.4	176.9

Fig. 4 shows the k-eff (for the first eigenvalue problem) and k-src (for the second fixed-source problem) histories obtained with the original and optimized search algorithms for the first case. As can be seen in Table III, the total numbers of iterations (i.e., fuel cycle calculations) of the first case are 27 and 12 for the original search algorithm and

optimized search algorithm, respectively. As expected, the first calculated k-eff value obtained with the initial user-specified enrichment parameter in the optimized search algorithm is the same as the counterpart in the original search algorithm. However, the second k-eff value is different from that in the original search algorithm because the full external search is made in the optimized search algorithm while only one external cycle calculation is performed in the original search algorithm.

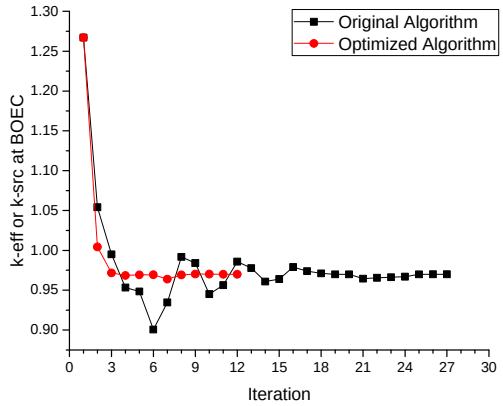

Fig. 4. k-eff and k-src histories of Case 1 obtained with original and optimized search algorithms.

Table IV compares the total number of equilibrium cycle calculations for both eigenvalue and fixed-source problems and the computational time obtained with the enhanced and optimized search algorithms for all the 50 cases. The average number of fuel cycle calculations at the final search level in the corresponding eigenvalue problem and the average numbers of fuel cycle calculations at the preliminary and final search levels in the fixed-source problem for the enhanced and optimized search algorithms are practically similar each other. However, the average value of the 50 cases for the number of fuel cycle calculations at preliminary search level in the corresponding eigenvalue problem is 13.92 for the enhanced search algorithm while that of the optimized search algorithm is 10.38. Relative to the enhanced search algorithm, the optimized search algorithm reduces the number of fuel cycle calculations at the preliminary search level in the corresponding eigenvalue problem by a factor of 1.3.

Fig. 5 shows the k-eff and k-src histories of the optimized search algorithm for the first two best (Case 41 and Case 39) and the first two worst (Case 21 and Case 40) cases. For Case 21 and Case 40, the k-eff values oscillated at the first several iteration steps due to the relatively large initial and second enrichment guesses. However, it is noted that k-src values converged within a total of 19 fuel cycle calculations and the numbers were competitive compared to the counterparts (i.e., 17) of the two best cases. These results showed that the performance of the optimized search algorithm is practically insensitive to the user-specified enrichment parameter guesses.

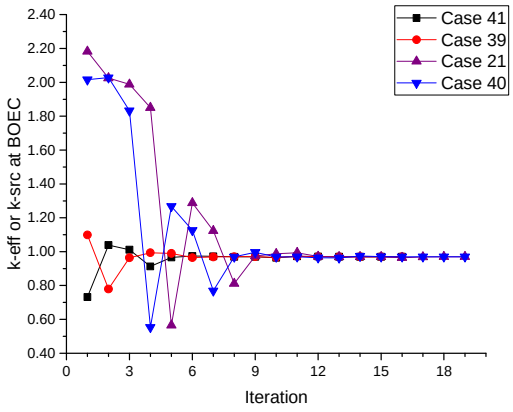

Fig. 5. k-eff and k-src histoies obtained with the optimized search algorithm of the first two best and the first two worst cases.

IV. CONCLUSIONS

An enhanced search algorithm for the charged fuel enrichment in the equilibrium cycle analysis of REBUS-3 has been developed to minimize the dependency on the user-specified enrichment parameters [4]. This enhanced search algorithm has been further optimized to reduce the computational time and the dependency on the initial guesses for fixed-source equilibrium cycle problems by minimizing the number of flux calculations using a partial convergence of equilibrium cycle calculations in the enrichment search for the corresponding eigenvalue problem of the fixed-source problem.

Using an 840 MWt ADS blanket design, a series of sensitivity analyses were performed for a fixed-source equilibrium cycle problem with 50 randomly generated pairs of user-specified enrichment parameters. Numerical results showed that the optimized search algorithm is able to produce a converged solution even when the user-specified initial guesses are far from the converged solution and reduce the number of flux calculations relative to the original and enhanced search algorithms. In practice, numerical results showed that the optimized search algorithm could reduce the number of flux calculations by a factor of 1.6 and 1.2, respectively, compared to the original and enhanced algorithms.

Table IV. Total Number of Equilibrium Cycle Calculations for Both Eigenvalue and Fixed-Source Problems and Computational Time Obtained with Enhanced and Optimized Algorithms

Case No.	Search Algorithm									
	Enhanced					Optimized				
	Number of fuel cycle calculations				Time, sec	Number of fuel cycle calculations				Time, sec
	k-eff		Source			k-eff		Source		
	Prelim.	Final	Prelim.	Final		Prelim.	Final	Prelim.	Final	
1	7	1	5	1	157	5	1	5	1	149
2	11	1	5	1	180	9	1	6	1	183
3	12	1	6	1	198	10	1	6	1	190
4	10	1	6	1	184	8	1	5	1	167
5	10	1	5	1	172	8	1	6	1	176
6	10	1	5	1	177	8	1	6	1	181
7	8	1	5	1	161	6	1	6	1	162
8	11	2	7	1	204	7	2	5	1	173
9	11	1	5	1	181	10	1	6	1	188
10	13	1	6	1	204	11	1	5	1	187
11	15	1	6	1	216	12	1	5	1	197
12	15	1	6	1	219	13	1	5	1	204
13	20	1	6	2	266	14	1	2	2	205
14	15	1	5	1	204	12	1	6	1	203
15	18	1	5	1	227	15	2	7	1	242
16	15	1	5	1	207	13	1	2	2	200
17	10	1	5	1	174	8	1	6	2	190
18	10	1	5	1	176	8	1	6	1	179
19	10	1	6	1	182	8	1	6	1	177
20	10	1	5	1	172	8	1	4	1	171
21	27	2	7	1	313	14	1	3	1	175
22	19	1	6	1	243	12	1	5	1	196
23	17	1	5	1	218	16	1	6	1	235
24	16	1	5	1	215	14	1	5	1	210
25	21	1	6	1	261	16	1	5	1	230
26	26	1	5	1	284	12	1	5	1	196
27	12	1	6	1	196	7	2	5	1	175
28	20	1	6	2	264	14	1	4	1	197
29	18	1	6	2	254	14	1	4	1	200
30	4	2	4	2	184	4	1	5	1	147
31	9	1	5	1	167	8	1	6	1	175
32	22	2	4	2	291	12	2	7	1	220
33	15	1	5	1	205	13	1	2	2	198
34	14	1	5	1	195	12	1	5	1	190
35	11	1	5	1	180	9	1	6	2	197
36	22	1	5	1	260	17	1	5	1	232
37	10	1	5	1	174	6	2	5	1	167
38	10	2	7	1	197	8	1	5	1	169
39	10	1	6	1	180	8	1	6	1	176
40	21	1	6	2	275	8	3	7	1	211
41	10	1	6	1	182	8	1	6	1	176
42	15	1	6	1	216	13	1	6	1	210
43	25	1	6	1	287	16	1	5	1	223
44	10	1	5	1	177	8	1	6	2	194
45	16	1	5	1	211	13	1	5	1	199
46	9	2	4	2	203	7	2	5	1	166
47	13	1	6	1	203	10	1	5	1	184
48	13	1	5	1	191	11	1	5	1	184
49	10	2	7	1	197	8	1	6	1	180
50	10	1	5	1	174	8	1	4	1	157
Avg.	13.92	1.14	5.46	1.14	209.2	10.38	1.16	5.18	1.12	189.9

REFERENCES

1. B. J. TOPPLE, “A User’s Guide to the REBUS-3 Fuel Cycle Analysis Capability,” ANL-83-2, Argonne National Laboratory (1983).
2. W. S. YANG and B. J. TOPPLE, “REBUS-3 Code Enhancements for ADS Fuel Cycle Analyses,” ANL-AAA-016, Argonne National Laboratory (2002).
3. R. P. HOSTENY, “The ARC System Fuel Cycle Analysis Capability, REBUS-2,” ANL-7721, Argonne National Laboratory (1978).
4. T. K. PARK, W. S. YANG, and S. J. KIM, “An Enhanced Search Algorithm for the Charged Fuel Enrichment in Equilibrium Cycle Analysis of REBUS-3,” *Annals of Nuclear Energy*, **103**, 17 (2017).
5. W. S. YANG and H. S. KHALIL, “Analysis of the ATW fuel cycle using REBUS-3 code system,” *Trans. Am. Nucl. Soc.*, **81**, 277 (1999).
6. C. S. LIN, T. K. PARK, and W. S. YANG, “Fast Reactor and Accelerator Driven System Core Design Studies for Two-Stage Fast Spectrum Fuel Cycle Option,” *Nuclear Technology*, **197**, 29 (2017).
7. T. K. PARK, C. S. LIN, and W. S. YANG, “A Moderated Target Design for Minor Actinide Transmutation in Sodium-Cooled Fast Reactor,” *Annals of Nuclear Energy*, **98**, 178 (2016).
8. R. D. LAWRENCE, “The DIF3D Nodal Neutronics Option for Two- and Three-Dimensional Diffusion Theory Calculations in Hexagonal Geometry,” ANL-83-1, Argonne National Laboratory (1983).
9. K. L. DERSTINE, “DIF3D: A Code to Solve One-, Two-, and Three-Dimensional Finite Difference Diffusion Theory Problem,” ANL-82-64, Argonne National Laboratory (1984).
10. NEA, “Comparison Calculations for an accelerator-driven Minor Actinide burner,” Nuclear Energy Agency, NEA/NSC/DOC(2001)13.
11. C. H. LEE and W. S. YANG, “MC2-3: Multigroup Cross Section Generation Code for Fast System Analysis,” ANL/NE-11-41, Argonne National Laboratory (2011).