The Sandwich Method for Determining Source Convergence in Monte Carlo Calculation

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In slow convergence problems, it is difficult to ascertain whether the source iteration has converged or not. So far, in Monte Carlo calculations, there is no good way to know how many skip batches are required to obtain the correct source distribution. In order to solve this problem, we have proposed a new "sandwich method" for cases of slow source convergence, which was presented in the ANS winter meeting in 2002. In this report, we proposed a method to determine the most important region for using sandwich method. Meanwhile, we have applied the sandwich method to four benchmark problems proposed by the source convergence group of the OECD/NEA Working Party of Nuclear Criticality Safety.

KEYWORDS: Sandwich method, Monte Carlo calculation, slow source convergence.

1. Introduction

In slow convergence problems, it is difficult to ascertain whether the source iteration has converged or not. Although the source distribution appears to have essentially reached stability after a number of batches of source iteration, the distribution of fission neutrons may still remain quite different from the ultimate one. Thus, the neutron keff values found up to this point need to be further proved. So far, in Monte Carlo calculations, there is no good way to know how many skip batches are required to obtain the correct source distribution. In order to solve this problem, we have proposed a new "sandwich method" for cases of slow source convergence, which was presented in the ANS winter meeting in 2002. The essence of this method is that a final, converged eigenvalue keff is approached starting from both higher and lower eigenvalues. In general, a lower eigenvalue estimate for the first active cycle can be obtained by assuming a flat uniform source. With further source iterations, keff will increase gradually for every active cycle. On the other hand, if the initial source is assumed to be confined at the most important region, then a higher estimate of keff will accrue for the first active cycle, and keff will decrease gradually for each subsequent cycle. A final, converged eigenvalue keff should fall between these two trend curves. In this report, we proposed a method for determining the most important region in source iteration. Meanwhile, we have applied the sandwich method to four benchmark problems proposed by the source convergence group of the OECD/NEA Working Party of Nuclear Criticality Safety.

2. A method for determining the most important region in source iteration

We will call the region where neutrons generate the most progenies the most important region. Concentrating the source in this region will create a higher eigenvalue for the first cycle. To find such an important region, calculations are separately performed with a uniform initial source distribution in each region. The keff's obtained from one active cycle calculations are compared. The region whose source gives the highest estimate value of keff after one cycle calculation will be the most important region. If the initial source is assumed to be concentrated only in that region, the eigenvalue will have a higher value and will gradually decrease with source iterations toward the converged keff value.

3. Benchmark calculations [1)]

To verify the efficiency of the sandwich method, it has been applied to the following benchmark problems. keff calculations are performed with two types of initial source, a uniform source and an important region source as defined above. keff values for source iteration cycles will gradually increase for the uniform source and will gradually decrease for the important region source. When the difference of keff values obtained from the two source conditions becomes less than a chosen limiting value, the source iteration is assumed to be converged. And iterations before that convergence point are to be skipped. keff calculations will continue, then, with a merged convergence source until the standard deviation becomes sufficiently small.

3.1 OECD/NEA Source Convergence Benchmark 1: Checkerboard storage of assemblies

The model comprises a notional 24x3 LWR fuel storage rack with duel elements stored in alternate locations. The fuel elements are ~5% enriched-by-weight fuel elements located within fully water-flooded steel storage racks surrounded by a close-fitting full concrete reflection on three sides, water on the remaining side and water on the top and bottom. The fuel elements are formed from a 15x15 lattice of Zr-clad UO2. The calculation configurations are shown in Figs. 3.1.1(a-b).

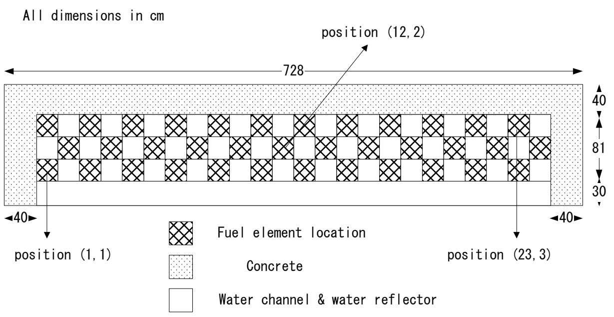

Fig.3.1.1(a) Horizontal cross section of the problem geometry for benchmark 1.

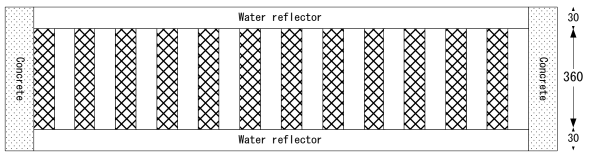

Fig.3.1.1(b) Vertical cross section of the problem geometry for benchmark 1.

In order to obtain the most important region for the problem, criticality calculations have been carried out using one active plus 0 skip cycles with 100000 particles. The initial source is sampled uniformly in each fuel assembly. The keff's are shown in Table 3.1.1. From Table 3.1.1, we may conclude that the fuel assembly in position (1,3) is the most important region.

Table 3.1.1 keff's obtained from one active cycle with 100000 particles.

	1	2	3	4	5	6
3	0.87784		0.87249		0.87252	
2		0.87294		0.87320		0.87320
1	0.86429		0.86034		0.86034	

	7	8	9	10	11	12
3	0.87252		0.87252		0.87252	
2		0.87320		0.87320		0.87320
1	0.86034		0.86034		0.86034	

	13	14	15	16	17	18
3	0.87252		0.87252		0.87252	
2		0.87320		0.87320		0.87320
1	0.86034		0.86034		0.86034	

	19	20	21	22	23	24
3	0.87252		0.87252		0.87177	
2		0.87320		0.87324		0.87194
1	0.86034		0.86034		0.86004	

Next, critical calculations are performed with two different initial source guesses. The uniform source is sampled uniformly within all fuel assemblies. On the other hand, the important region source is sampled uniformly only within fuel assembly in position (1,3). The initial guess for keff is set to 1.0, while number of particles per cycle is set to 20000. The computed keff results obtained from 1000 active cycles and 0 skip cycles are shown in Fig.3.1.2.

It can be seen that the source convergence is very slow, however, as shown in this figure, we may conclude that the final, converged keff lies between the upper and lower trend curves.

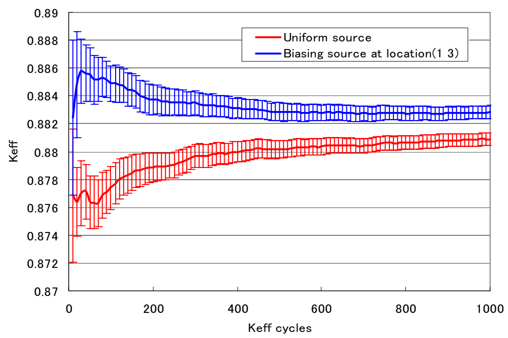

Fig.3.1.2 keff V.S. the keff cycles using sandwich method with two initial source distributions for benchmark 1.

3.2 OECD/NEA Source Convergence Benchmark 2: Pincell array with irradiated fuel

This benchmark problem is a modified version of the OECD/NEA burnup credit criticality benchmark (Phase IIA effect of axial burnup profile) which are published in JAERI-Research 96-003 (NEA/NSC/DOC(96)01). The aim is to study source convergence problems associated with the axial burnup profile (end effect). The calculation configuration is shown in Fig. 3.2.1. Fuel region identification of each region for Case2_3 in Benchmark 2 is given in Table 3.2.1.

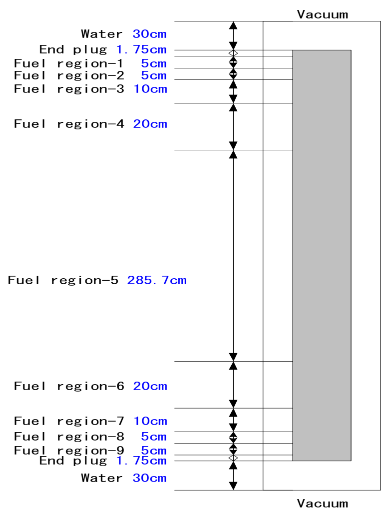

Fig. 3.2.1 vertical cross section of the problem geometry for benchmark 2.

Tab.3.2.1 Fuel region identification for Case2_3.

Region	1	2	3	4	5
Fuel-type	B21G	B24G	B30G	B40G	B55G

Region	6	7	8	9
Fuel-type	B40G	B30G	B30G	B24G

The composition of LWR spent fuel consists of low burnup, more reactive end regions separated by a long, less active, high burnup part. Moreover, there is only a slight difference in composition between the upper and lower ends for Case2_3. In order to obtain the most important region for Case2_3, we have investigated the problem by assuming the pincell includes three parts: Upper end region, middle region and lower end region. Criticality calculations were performed with specific initial source sampled uniformly in each part. The keff's obtained from one active plus 0 skip cycles with 100000 particles are shown in Table 3.2.2. From the Table 3.2.2, we may conclude that the upper end region is the most important region.

Table 3.2.2 keff's obtained from one active cycle with 100000 particles for Case2_3.

	keff
Upper end region	1.07294
Middle region	0.98192
Lower end region	1.06705

Moreover, considering the upper end region includes four burnup regions with different atomic density, we may further investigate the problem to obtain the most reactive region among these four burnup regions. Criticality calculations were performed with specific initial source sampled uniformly in each region. The keff results are shown in Table 3.2.3. In Table 3.2.3, we now see that the region 3 is the most reactive region.

Table 3.2.3 keff's obtained from one cycle for the upper four regions.

	Keff
Region 1	0.91581
Region 2	1.07590
Region 3	1.13078
Region 4	1.08257

Critical calculations for Case2_3 are performed using the sandwich method with two initial source distributions. The uniform source is sampled uniformly over the volume of the pin pellet, while the important region source is confined uniformly sampling at the more reactive upper end region. The initial guess for keff is set to 1.0, while number of particles per cycle is set to 20000. The computed keff results obtained from 1000 active cycles and 0 skip cycles are shown in Fig.3.2.2. Furthermore, we now limit the important region source at the most reactive region 3 in order to compare the trend of convergence with different important region. The results are shown in Fig.3.2.3.

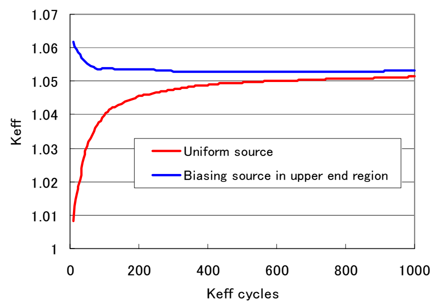

Fig.3.2.2 keff V.S. the keff cycles using sandwich method with two initial source distributions for Case2_3.

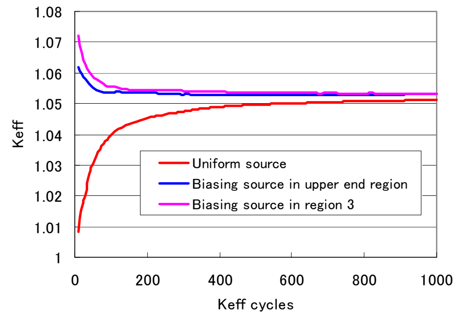

Fig.3.2.3 Comparison of keff's versus the keff cycles using different biasing source for Case2_3.

3.3 OECD/NEA Source Convergence Benchmark 3: Three thick one-dimensional slabs

This benchmark problem is composed of one-dimensional infinite slab geometry as shown in Fig. 3.3.1. A slab of water separates two fissile units. The thickness of unit 1 is fixed at 20cm. The thicknesses of unit 2 and water layer for the studied cases are given in Table 3.3.1.

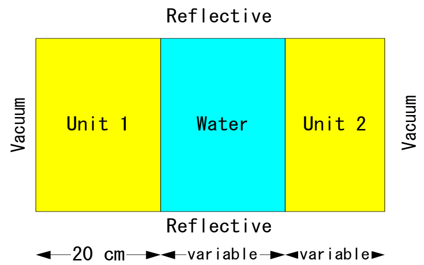

Fig.3.3.1 Configuration of coupling array.

Tab.3.3.1 Thickness of unit 1, unit 2 and water layer for the studied cases.

Case number	Thickness of Unit 1	Thickness of Unit 2	Water thickness
3_2	20cm	18cm	30cm
3_6	20cm	18cm	20cm
3_10	20cm	18cm	10cm
3_14	20cm	18cm	2cm
3_16	20cm	18cm	0cm

In order to obtain the most important region for the above cases, we first extend our consideration to the thickness of the water layer. Since the water layer is considerable thick for Cases 3_2, 3_6, and 3_10, the configuration can be considered as two loosely coupled asymmetrical fuel system. Therefore, the thicker fissile unit 1 can be treated as the most important region. On the other hand, since the water layer thickness is only 2cm for Case 3_14 and 0cm for Case 3_16, the configuration can't be considered as a loosely coupled system. To obtain the most important region for cases 3_14 and 3_16, the unit 1 and 2 is split into 8 regions as shown in the Fig. 3.3.2. Criticality calculations were performed with specific initial source sampled uniformly in each region. The keff's obtained from one active plus 0 skip cycles with 100000 particles are shown in Table 3.3.2. From Table 3.3.2, we may conclude that the region 4 is the most important region for both Case 3_14 and Case 3_16. Meanwhile, the unit 1 and 2 can be also split into 8 regions for Cases 3_2, 3_6, and 3_10 to obtain a more noticeable important region. Criticality calculations were performed for Case 3_6. From Table 3.3.2, we can see that the region 3 is the most important region for Case 3_6.

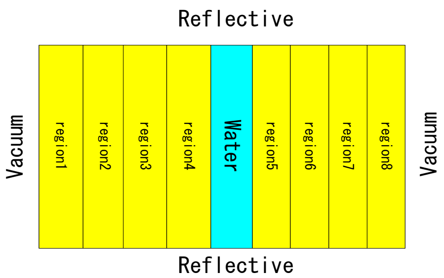

Fig.3.3.2 Calculation configuration for Cases 3_14 & 3_16.

Table 3.3.2 keff's obtained from one cycle with 100000 particles for Cases 3_6, 3_14, and 3_16.

	Keff Case 3_6	Keff Case 3_14	Keff Case 3_16
Region 1	0.61012	0.62463	0.62737
Region 2	0.97777	1.01671	1.02366
Region 3	1.05041	1.16588	1.18590
Region 4	0.88889	1.19076	1.23411
Region 5	0.86106	1.17857	1.22697
Region 6	1.00372	1.13601	1.16185
Region 7	0.92045	0.97437	0.98402
Region 8	0.57963	0.60078	0.60510

Critical calculations for the above cases are performed using the sandwich method with two initial source distributions. The uniform source is sampled uniformly between the unit 1 and unit 2. The important region source, i.e. biasing source, is restrained uniformly sampling at the unit 1 for Cases 3_2, 3_6, and 3_10, while, the important region source is confined uniformly sampling at the more reactive region 4 for Cases 3_14 and 3_16. The initial guess for keff is set to 1.0, while number of particles per cycle is set to 20000. The computed keff results obtained from 1000 active cycles and 0 skip cycles are shown in Fig.3.3.3 ~ Fig.3.3.7.

For Cases 3_2, 3_14 and 3_16, comparison of keff's versus the keff cycles using different biasing source are shown in the following as well.

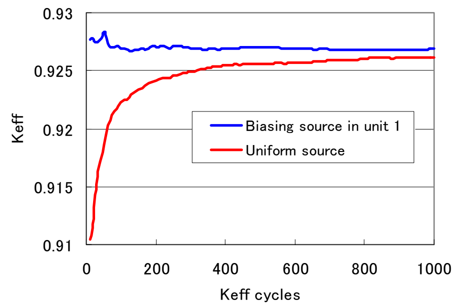

Fig.3.3.3 keff V.S. the keff cycles using sandwich method with two initial source distributions for Case 3_2 .

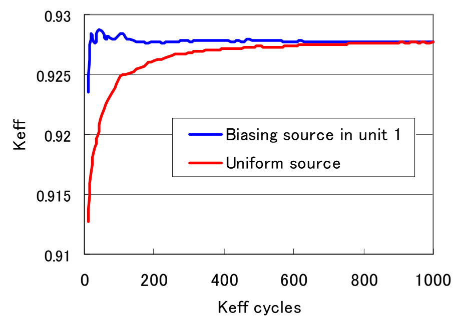

Fig.3.3.4(1) keff V.S. the keff cycles using sandwich method with two initial source distributions for Case 3_6 .

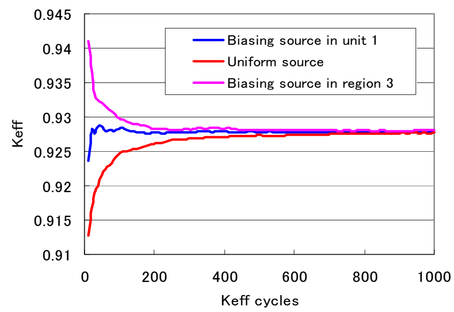

Fig.3.3.4(2) Comparison of keff's versus the keff cycles using different biasing source for Case3_6.

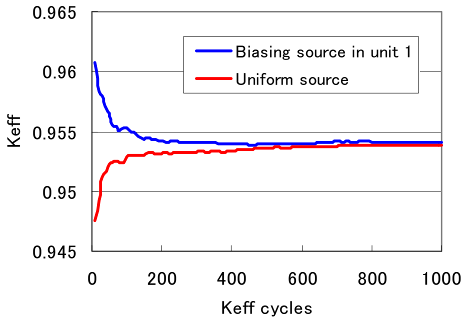

Fig.3.3.5 keff V.S. the keff cycles using sandwich method with two initial source distributions for Case3_10.

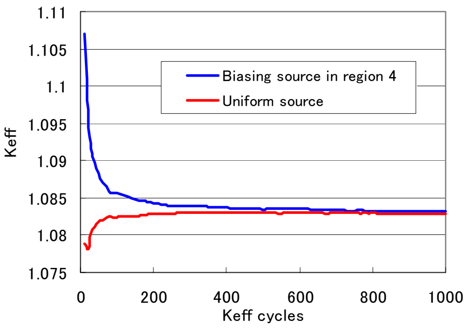

Fig.3.3.6(1) keff V.S. the keff cycles using sandwich method with two initial source distributions for Case3_14 .

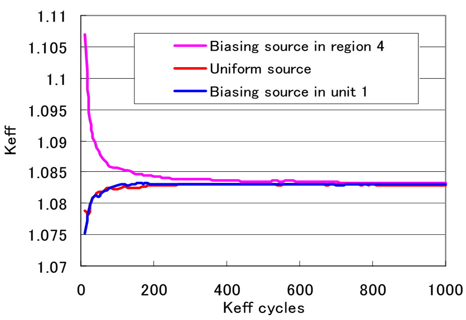

Fig.3.3.6(2) Comparison of keff's versus the keff cycles using different biasing source for Case3_14 .

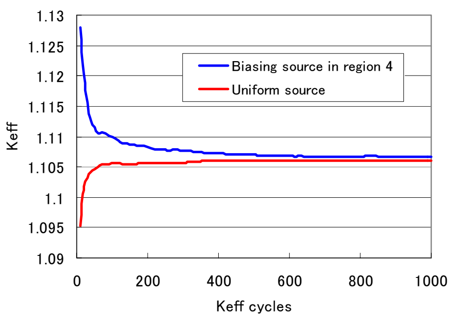

Fig.3.3.7(1) keff V.S. the keff cycles using sandwich method with two initial source distributions for Case3_16 .

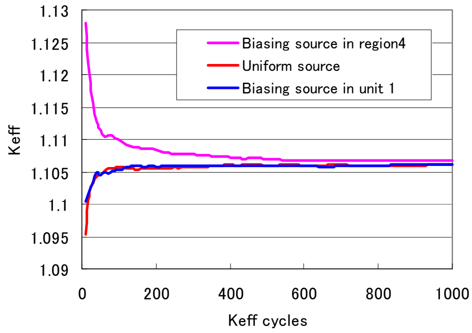

Fig.3.3.7(2) Comparison of keff's versus the keff cycles using different biasing source for Case3_16.

3.4 OECD/NEA Source Convergence Benchmark 4: Array of interacting spheres

In this benchmark a lattice of 5x5x1 separated highly enriched uranium metal sphere is considered. The separating material is air. The center-to-center distance between spheres is 80cm. The radius of the central sphere is 10cm while the radius of the other sphere is 8.71cm. Figure 3.4.1 describes the overall geometry. The benchmark is an adaptation from Kadotani et al. (Proc.ICNC91, Oxford, 1991).

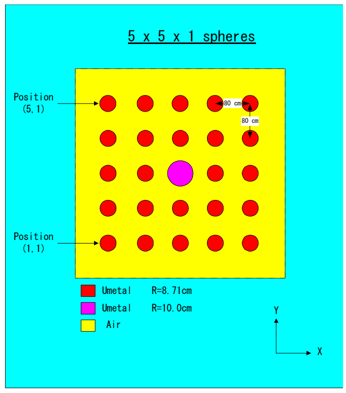

Fig.3.4.1 Calculation geometry for the benchmark 4.

Since the overall geometry is symmetric, we may investigate one-eighth of spheres to obtain the most important region. Meanwhile, the central sphere is split into two parts: an inner 5cm radius sphere and the outer 5cm thick surroundings. The central sphere is in position (3,3). Accordingly, the central point of the sphere is named position (3,3,0); the inner 5cm radius sphere is named position (3,3,1); and the outer 5cm thick surroundings is named position (3,3,2).

Criticality calculations were performed with specific initial source sampled uniformly in each region. The keff's obtained from one active plus 0 skip cycles with 100000 particles are shown in Table 3.4.1. From Table 3.4.1, we may conclude that the position (3,3,1) is the most important region. And the central point (3,3,0) is the most important point.

Table 3.4.1 keff's obtained from one active cycle with 100000 particles for benchmark 4.

	keff
Position (1,1)	0.90366
Position (1,2)	0.90759
Position (1,3)	0.90754
Position (2,2)	0.91252
Position (2,3)	0.91318
Position (3,3)	1.01032
Position (3,3,0)	1.49746
Position (3,3,1)	1.40099
Position (3,3,2)	0.95590

Critical calculations for the above cases are performed using the sandwich method with two initial source distributions. The uniform source is sampled uniformly over all the 25 spheres. The important region initial source, i.e. biasing source, is sampled uniformly in the inner 5 cm radius sphere (3,3,1). The initial guess for keff is set to 1.0, while number of particles per cycle is set to 20000. The computed keff results obtained from 1000 active cycles and 0 skip cycles are shown in Fig.3.4.2.

Finally the important region source is confined at the most important point (3,3,0) in order to compare the trend of convergence between the important region and the important point. From Fig.3.4.3, we see that there is no significant difference between the keff results obtained from the important region and the important point. Therefore, we may conclude that both the important region and the important point would be adequate for the problem when the sandwich method is adopted.

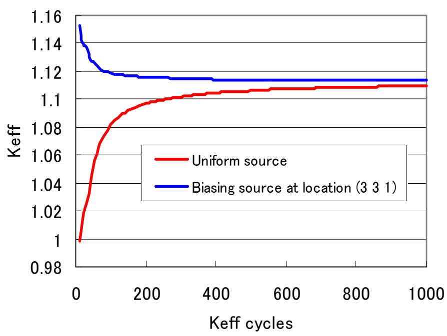

Fig.3.4.2 keff V.S. the keff cycles using sandwich method with two initial source distributions for benchmark 4.

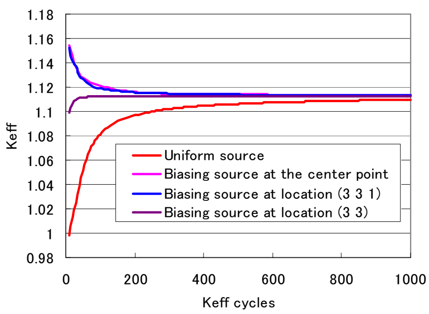

Fig.3.4.3 Comparison of keff's versus the keff cycles using different biasing source for benchmark 4.

4. Concluding Remarks

We have applied the sandwich method to the four OECD/NEA benchmark problems on source convergence. The upper limit for keff is obtained by assuming initial source to be confined at the most important region. The most important region can be obtained by comparing the keff results from the 1st cycle calculation. As for the benchmark No.1, the location (1 3), i.e., top left-hand fuel assembly, is the most important region; for the benchmark No.2, the region 3 is the most important region; for the benchmark No.3, the region 3 is the most important region for Case3_6, while, the region 4 is the most important region for Case3_14 and Case3_16; for the benchmark No.4, the location (3, 3, 1), i.e., the inner 5cm radius sphere, is the most important region.

In benchmark No.4, if the biasing source is assumed to be confined at the central 10cm radius sphere (3,3), the keff obtained from the 1st cycle shows lower than the converged one. This means that the importance of the central sphere is less than the average importance of the whole system. However, the importance of the central point (3,3,0) and the importance of the central region (3,3,1) are higher than the average one. So, if initial biasing source is assumed to be confined at such a point or region, a higher keff can be obtained from the 1st cycle calculation.

The calculation results obtained from the above benchmark problems show that the "Sandwich Method" is an effective means for criticality safety evaluation.

References

1) R.N. Blomquist (ANL), A. Nouri (OECD NEA-France), " The OECD/NEA Source Convergence Benchmark Program," TANSAO 87 1-586 (2002).