

## Hybrid Method of MOC and $S_N$ Nodal for PWR Core Analysis

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### ABSTRACT

A hybrid method of MOC and  $S_N$  nodal has been developed to accurately calculate the 3-D pin by pin power distribution. Assembly calculations are performed based on MOC by using the albedo boundary condition calculated by a 3-D core calculation which uses cell-averaged cross sections obtained from the assembly calculations. The proposed method has been applied to the 2-D and 3-D C5G7 benchmark problems. From the numerical results, it was found that the proposed method improved the calculation accuracy compared to the conventional once-through method.

*Key Words:* PWR core, Method of characteristics, Cell homogenization,  $S_N$  nodal, Neutron leakage

### 1. INTRODUCTION

Recently whole core transport calculations are widely used so as to meet future requirements to come up with the next generation core design. The pin-by-pin transport capability will be necessary for evaluation of the next generation core because the heterogeneity of fuel assembled becomes strong. As the next generation core calculation method, we proposed "On Flight" (hereafter, referred the on-flight) calculations [1] by combining the two dimensional cell-heterogeneous transport calculation for generating cell average constants and three dimensional cell-homogenous pin-by-pin core calculations. The advantage of this method is to generate neutronic constants by considering the whole core calculations. Using the boundary condition obtained from the core simulator instead of the reflective boundary which is usually assumed in the current methodology, the assembly calculations with MOC [2] provide accurate cell constants including SPH factors to three dimensional  $S_N$  nodal transport code [3]. With the cell homogenized cross sections and the SPH factors, the cell homogeneous whole core calculation has the same accuracy as heterogeneous pin-by-pin calculation. Note that the cell homogenized cross sections and the SPH factors are generated with the method which authors established as the leakage dependent SPH method [4].

### 2. THEORY

The whole core calculations by using the three dimensional  $S_N$  nodal transport theory needs cell homogenized cross sections. The homogenization problem have already solved by using the

SPH factor [5] [6]. With the SPH factors, the calculation has good accuracy comparable to the pin by pin heterogeneous transport calculations. For reader's convenient, brief explanation is given.

The conventional SPH factors have established in the reflective boundary condition. If leakage exists at boundary, the commonly used SPH method doesn't work. This is because without the leakage preservation, the reaction rates can not be preserved.

In the case of albedo boundary case, the magnitude of in- and out-going current can not be determined. To avoid the problem, we introduced the balance equation to maintain net neutron current by changing the albedo [4]. The albedo is updated by repeating homogeneous assembly calculations by using the relation,

$$\beta^{(m)} = 1 - (1 - \beta) J_{out} / \bar{J}_{out}^{(m)} \quad (1)$$

where,  $\beta$  and  $J_{out}$  denote the albedo and the outgoing neutron current from a heterogeneous assembly calculation, and  $\bar{J}_{out}^{(m)}$  is the outgoing neutron current for the m-th iteration of homogeneous assembly calculations.  $\beta^{(m)}$  is the leakage dependent SPH factors. The convergence of  $\beta^{(m)}$  is very rapid, and only a few iteration is required to obtain the converged

In this chapter, the on-flight method is described and assembly calculation and core calculation solver used in the on flight method are mentioned.

## 2.1. On Flight Method (Hybrid Method)

Actual calculation procedure of the on flight method is summarized below;

- (i) First, homogeneous cell constants and SPH factors are generated by each single assembly model with reflective boundary condition.
- (ii) Using the cell constants and SPH factors obtained in step (i), a homogeneous core calculation is performed, in which each cell is homogenized (This is the same procedure as conventional homogeneous core simulation.)
- (iii) Boundary condition (albedo, current or surface flux) at assembly surface in the core simulation is evaluated. Here, the boundary condition is calculated for each cell surface along the assembly surface.
- (iv) Cell constants and SPH factors are generated again by each single assembly model with the albedo obtained in step (iii). In this calculation, the cell heterogeneity is, of course, considered.
- (v) Using the cell constants and SPH factors obtained in step (iv), the cell homogeneous core calculation is performed again. Iterations from step (iii) to (v) are continued until convergence of  $\beta^{(n)}$  is achieved.

The interference effect on the spectrum from the adjacent assemblies can be considered because the assembly calculation is carried out with the boundary condition obtained by the previous core calculation.

The SPH method is derived to preserve the cell reaction rates between the cell-heterogeneous and cell-homogeneous calculations. The leakage dependent SPH method is also applied to preserve cell reaction rates between heterogeneous and homogeneous system. This method

makes sure the neutron leakage consistency between heterogeneous and homogeneous assembly calculation. The calculation flow of the on-flight method is show in Fig.1.

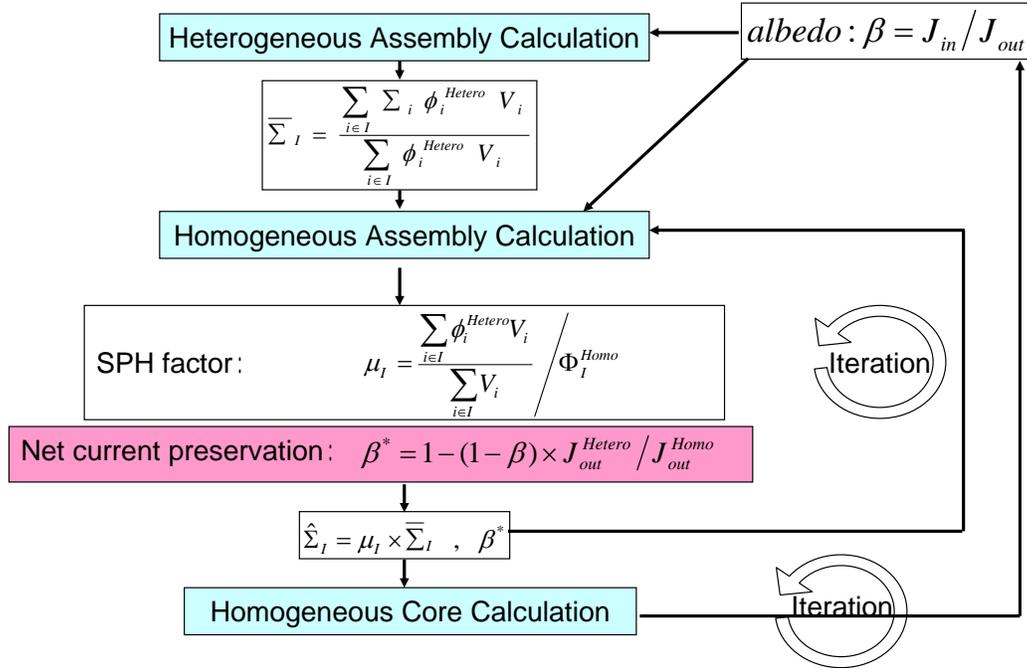


Figure.1 Calculation Flow

## 2.2. Assembly Calculation using Method of Characteristics

A two dimensional new heterogeneous MOC transport calculation code, GALAXY (Geometrically Arbitrary Lattice physics and Assembly calculation code in X-Y coordinate system) [1], [7] is being developed by Mitsubishi Heavy Industries, Ltd (MHI). In the on flight method, GALAXY performs each assembly calculation to provide cell constants. GALAXY has high flexibility in geometry modeling, e.g., irregularity in fuel rods array can be treated. Various types of mesh division for flat source approximation can be selected. In GALAXY, all geometrical models are treated by combination of circles, rectangles, lines and other primitive geometries. Although numbering of the flat source regions in MOC becomes cumbersome for complicated geometry, the factorial geometry [8] and the “R-function Solid Modeler” technique [9] successfully solved this problem.

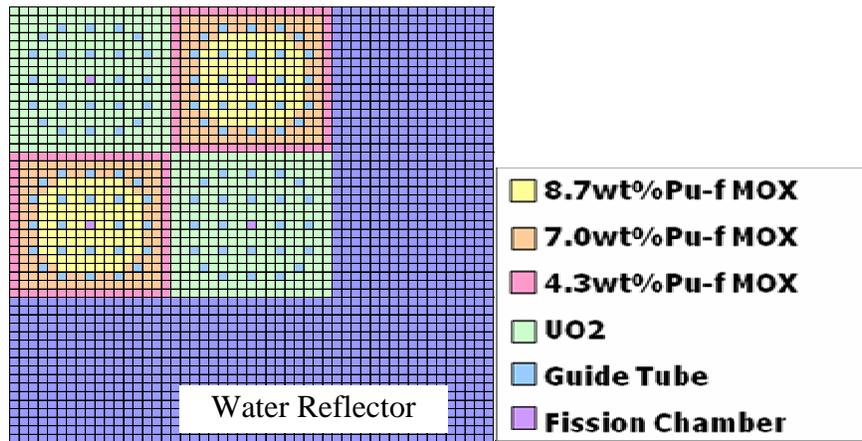
To connect core calculations and assembly calculations in the on flight method, the cell-wise energy dependent albedo condition is available in GALAXY. Coarse mesh finite difference (CMFD) method and parallel computing techniques are also applied to reduce the computation time. The parallelization of GALAXY is performed with MPI2.0. The inner iterations of angular flux are performed in parallel with each azimuthal decomposition group (angular

decomposition). In a typical 17x17 PWR assembly calculation, the parallel efficiency for the MOC solver with CMFD acceleration is about 80% on 12 processors.

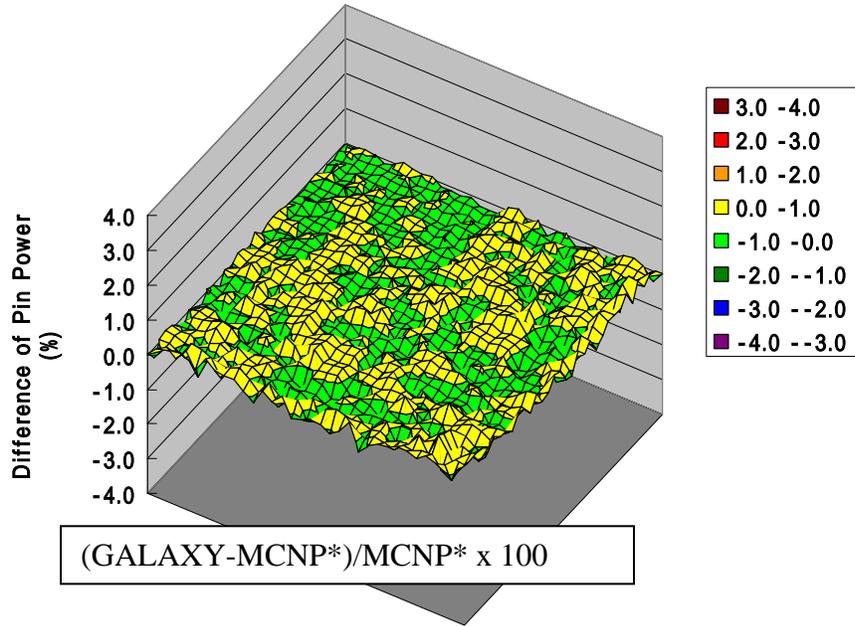
To validate GALAXY, 2D C5G7 benchmark problem [10] was analyzed. As for the discretization parameters for MOC, a path width of 0.05 cm was adopted, each  $\pi/2$  azimuthal segment was divided into 24 segments, a three-division polar angle set [11] was adopted. The calculation geometry is shown in Fig.2. The result was compared with MCNP [12] results using 300 million history [10]. The comparison of k-effective and pin-wise fission rate distribution is shown in Table 1 and Fig.3. It can be seen that GALAXY results agree very well with MCNP results. These results indicate that GALAXY has enough accuracy in the treatment of high heterogeneity.

**Table.1 Calculation results of 2-D C5G7 MOX benchmark problem. The reference results with MCNP were published.**

Code Name	K-eff	Error (pcm)	Max. Pin power	Error(%)	Min. Pin power	Error(%)	Max. error(%)	RMS Error(%)
Reference MCNP	1.18655	+/- 8	2.498	+/-0.16	0.232	+/-0.58	-----	0.34
GALAXY	1.18649	-5	2.498	-0.00	0.233	0.47	0.68	0.16



**Figure.2 Geometry of 2D-C5G7MOX benchmark.**



**Figure.3 Difference of pin power distribution between GALAXY and MCNP in UO<sub>2</sub> and MOX assemblies of 2D-C5G7 MOX benchmark.**

### 2.3. Pin-by-pin Core Calculation using Nodal S<sub>N</sub> Method

A three dimensional core calculation code, TECHXY has been developed by Osaka University [3]. In the on flight method, TECHXY works as pin-by-pin transport core simulator based on nodal S<sub>N</sub> method. In the transport calculation, each cell is homogenized.

Derivation of the three dimensional nodal S<sub>N</sub> equation is given here. The transport equation is described by

$$\sum_{c=x,y,z} \frac{\mu_c^m}{h_c} \frac{\partial \psi^m(x, y, z)}{\partial c} + \Sigma_t \psi^m(x, y, z) = Q^m(x, y, z) \quad (2)$$

where “*m*” is neutron direction of S<sub>N</sub> method,

$\Sigma_t$  is total cross section,

$\mu_c^m$  is cosine of neutron direction,

$Q^m$  is neutron source and

$h$  is node width.

We transform Eq. (2) to one-dimensional (*c*-coordinate) by integrating the remaining coordinates *c*' over each node to obtain

$$\frac{\mu_c^m}{h_c} \frac{\partial \psi^m(c)}{\partial c} + \Sigma_t \psi^m(c) = Q^m(c) - \sum_{c' \neq c} L_{c'}^m \quad (c = x, y, z). \quad (3)$$

$$= S^m(c),$$

The scalar flux, neutron source and leakage can be assumed to be expressed as polynomial expansion. Integrating Eq.(3) over a node, the angular dependent nodal equation is solved as follows:

$$\psi_{c\pm, out}^m = \frac{h_c}{\mu_c^m} \sum_{i=0}^2 S_i^m \int_{-1/2}^{1/2} f_i(\pm t) \exp\left[\frac{\Sigma_t h_c}{\mu_c^m} (t-1/2)\right] dt + \psi_{c\mp, in}^m \exp\left[-\frac{\Sigma_t h_c}{\mu_c^m}\right] \quad (c = x, y, z), \quad (4)$$

where  $f_i(t)$  is Legendre function,

“ $i$ ” is polynomial order,

$\psi_{c\pm, out}^m$  is outgoing angular flux on the node surface at  $t=+/-1/2$  and

$\psi_{c\pm, in}^m$  is incoming angular flux on the node surface at  $t=+/-1/2$ .

The  $f_i(t)$  satisfies the following normalization condition,

$$\int_{-1/2}^{1/2} f_i(t) f_j(t) dt = \delta_{i,j} = \begin{cases} 1 & (i = j) \\ 0 & (i \neq j) \end{cases}. \quad (5)$$

Next, nodal equivalent finite difference algorithm is derived. In order to keep the neutron balance in each node, the following neutron balance equation needs to be satisfied,

$$\sum_{c=x,y,z} \frac{\mu_c^m}{h_c} (\psi_{c+, out}^m - \psi_{c-, in}^m) + \Sigma_t \bar{\psi}^m = \bar{S}^m. \quad (6)$$

$\bar{\psi}^m$  and  $\bar{S}^m$  denote node averaged angular flux and neutron source considering transverse leakage, respectively. Using Eqs. (4) and (6), the node averaged angular flux is derived,

$$\bar{\psi}^m = \left( \sum_{c=x,y,z} \frac{\mu_c^m}{h_c a_{c+}^m} (b_{c+}^m \psi_{c-, in}^m + d_{c+}^m) + \bar{S}^m \right) / \left( \sum_{c=x,y,z} \frac{\mu_c^m}{h_c a_{c+}^m} + \Sigma_t \right) \quad (c = x, y, z). \quad (7)$$

where  $a_{c+}^m$ ,  $b_{c+}^m$  and  $d_{c+}^m$  are defined by:

$$a_{c+}^m = G_{c00+}^m / F_{x0+}^m$$

$$b_{c+}^m = \left( G_{c00+}^m + F_{c0+}^m G_{c0+}^m - \exp\left[-\frac{\Sigma_t h_c}{\mu_c^m}\right] G_{c00+}^m \right) / F_{c0+}^m, \quad (8)$$

$$d_{c+}^m = \sum_{j=1}^2 \left( G_{c0j+}^m - G_{c00+}^m F_{cj+}^m / F_{c0+}^m \right) S_{cj}^m$$

and,

$$F_{ci\pm}^m = \frac{h_c}{\mu_c^m} \int_{-1/2}^{1/2} f_i(\pm t) \exp\left[\frac{\Sigma_t h_c}{\mu_c^m} (t-1/2)\right] dt \quad (j = 0,1,2)$$

$$G_{ci\pm}^m = \int_{-1/2}^{1/2} f_i(\mp t) \exp\left[\frac{\Sigma_t h_c}{\mu_c^m} (t-1/2)\right] dt \quad (j = 0,1,2)$$

$$G_{cij\pm}^m = \frac{h_c}{\mu_c^m} \int_{-1/2}^{1/2} f_i(\pm t) \int_{-1/2}^t f_j(\pm t') \exp\left[\frac{\Sigma_t h_c}{\mu_c^m} (t'-t)\right] dt dt' \quad (i, j = 0,1,2)$$

In TECXHY, Eq. (7) is used to calculate node averaged angular fluxes. Equation (7) is similar to the conventional diamond difference equations used in  $S_N$  method, and the present method is easily implemented to the conventional  $S_N$  code.

CMFD is applied to TECXHY in order to reduce the computing time. The parallelization of TECHXY is also performed with MPI2.0. The inner iterations of angular flux are performed in parallel with angular decomposition. In 2D C5G7 calculation, the parallel efficiency of S6 calculation is about 90% on 6 processors.

### 3. NUMERICAL RESULTS

#### 3.1 Sn Quadrature order and Polynomial order

Let us first investigate the effect of orders of  $S_N$  quadrature and polynomials used in TECHXY. Table.2 shows the difference of k-effective and pin powers when varying the  $S_N$  quadrature and polynomials for the 2D C5G7 benchmark. Pin cells are homogenized and the cell pitch is 1.26cm. From the results, the  $S_N$  quadrature of 4 and the polynomial order of 2 is satisfactory.

**Table.2 Effect of  $S_N$  order and polynomial order of Nodal Expansion in C5G7 benchmark calculation**

Difference of k-eff [pcm]			
	N0	N1	N2
<b>S2</b>	-284	-24	-44
<b>S4</b>	-239	33	6
<b>S6</b>	-239	29	4
<b>S8</b>	-237	29	0*

R.M.S. Difference of Pin Power [%]			
	N0	N1	N2
<b>S2</b>	7.35	1.66	1.53
<b>S4</b>	6.38	0.32	0.16
<b>S6</b>	6.31	0.35	0.14
<b>S8</b>	6.28	0.37	0*

\* Reference Solution : S8, N2

Sx :  $S_N$  Order (2-8)

Nx: Polynomial Order of Nodal Expansion (0-2)

Table.3 shows the effect of node division in axial direction for the 3D C5G7 benchmark. Compared to the fine node of 5cm pitch, the calculation using the node width of 10cm is satisfactory. So, we use the 10cm node width as shown in Fig.4.

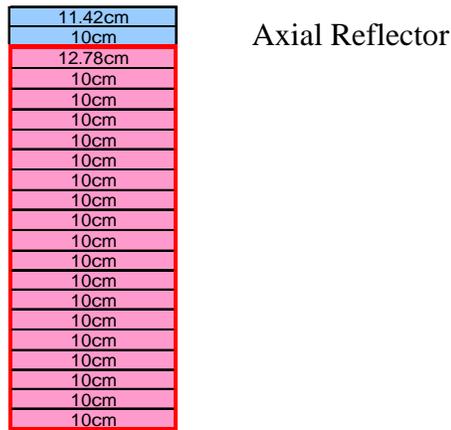
**Table.3 Effect of Z axial node width in C5G7 benchmark calculation**

Axial Node Width [cm]	Difference of k-eff[pcm]	R.M.S. Difference of Pin Power[%]
20	22	0.09
10	4	0.01
5	0*	0*

\* Reference Solution : 5cm

S<sub>N</sub> Order : 8

Polynomial Order of Nodal Expansion : 2



**Figure.4 Node division in the axial direction in 3D C5G7 benchmark calculation**

The effect of S<sub>n</sub> quadrature and polynomial order for the 3-D benchmark is shown in Table.4. Here the conclusion drawn from the 2-D benchmark is still valid: The S<sub>N</sub> quadrature order of 4 and the polynomial order of 2 is satisfactory.

**Table.4 Effect of S<sub>N</sub> order and polynomial order of Nodal Expansion in 3-D C5G7 benchmark calculation**

Difference in k-effective[pcm]			R.M.S. Difference in Pin Power[%]		
	N1	N2		N1	N2
S4	34	5	S4	0.33	0.17
S6	31	4	S6	0.36	0.14
S8	30	0*	S8	0.38	0*

\* Reference Solution : S8, N2

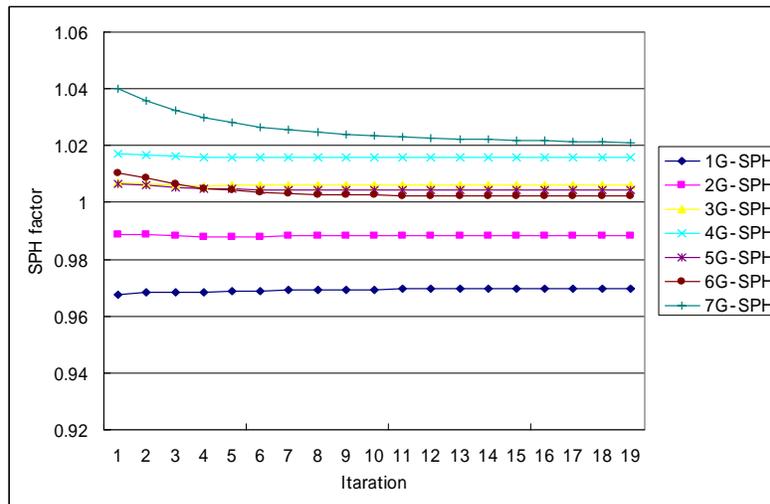
S<sub>x</sub> : S<sub>n</sub> Order(4-8)

N<sub>x</sub> : Polynomial Order of Nodal Expansion(1-2)

### 3.2 2-D C5G7 Benchmark Results

The proposed hybrid method was first applied to the 2-D C5G7 benchmark problem, where UO<sub>2</sub> and MOX assemblies are surrounded by a water reflector.

For the assemblies adjacent to different type fuel assemblies, the water reflectors and those having a corner reflector, we have used the assembly model with different type fuel cells and water reflector of 2 cell width. Using this model, the SPH factors and the albedo were successfully converged as shown in Fig.6.



**Figure.6 Convergence of SPH factor for 2-D C5G7 benchmark problem (Surface cell of MOX assembly)**

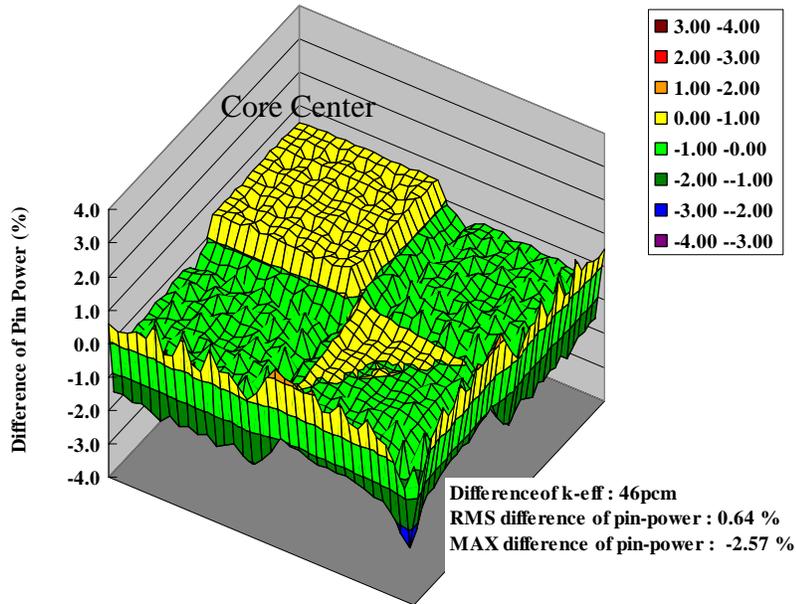
Using the obtained SPH factors, a core calculation was performed by the  $S_N$  nodal method.

The reference was calculated by the MOC method applied to the whole 2-D core. The azimuthal angle was divided into 16 for 90° degree, the polar angles divided into 3 using the TY method, and the path width was set to 0.05cm.

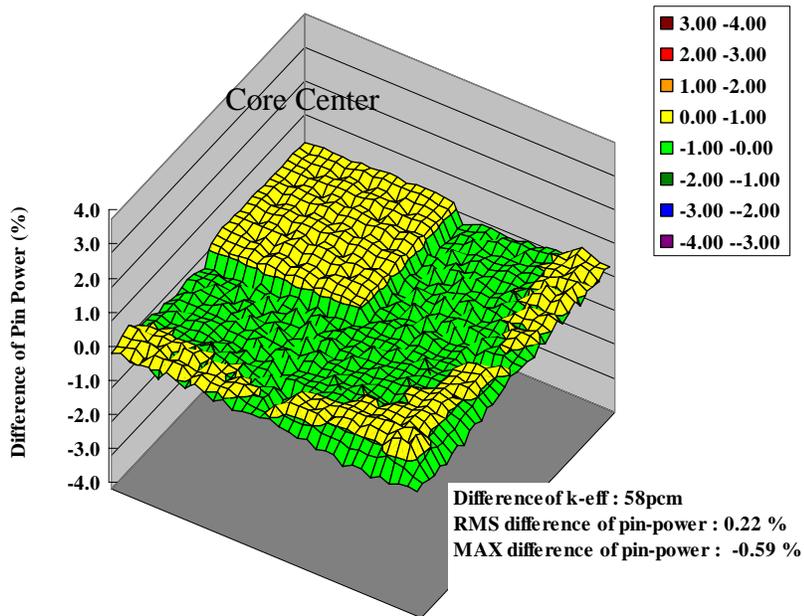
The comparison of  $k$ -effective and pin power results for the conventional method and the present methods with the reference MOC heterogeneous calculation result is shown in Figure.7. The conventional method uses homogeneous cross-sections obtained from each single assembly calculation with the reflective boundary condition.

The relative errors of  $k$ -effective are not significant in both methods. The relative percent error of pin power is reduced within 1% for the present method, and the maximum difference from the reference is also reduced to 0.6% from 2.6%. Thus it is found that the present method has enough accuracy.

### Conventional Method



### Present Method



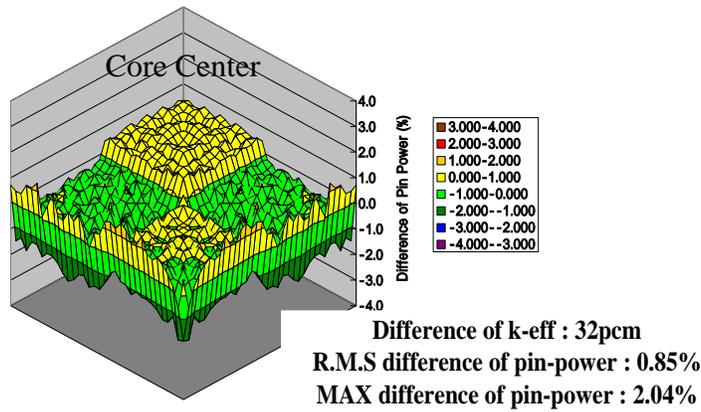
**Figure.7 Difference of k-effective and pin-power in the conventional method and the present method for 2-D C5G7 benchmark problem**

### 3.3 3-D C5G7 Benchmark Results

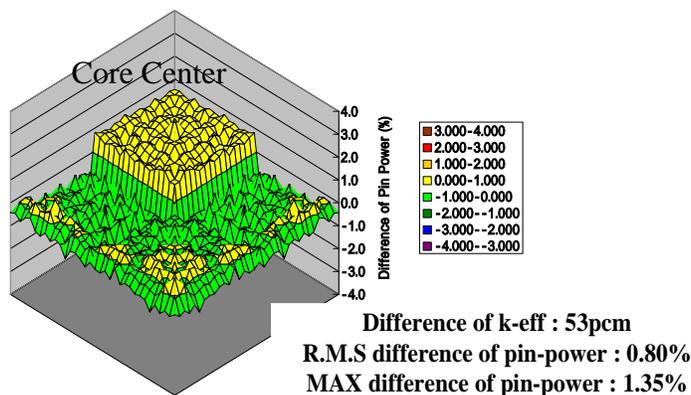
To check the accuracy of the proposed hybrid method in a 3-D core, we have applied it to the 3-D C5G7 benchmark. The reference calculation was performed by the Monte-Carlo MCNP code. The results of once-through method and the proposed method were compared with the reference one. The  $k_{eff}$  calculated by MCNP is 1.18381, and the difference from this result is 32pcm and 53pcm for the once-through method and the proposed method, respectively. The difference for the pin power (axially integrated power) is shown in Figure.8

The RMS difference was 0.85% and 0.80%, and the maximum power difference was 2.04% and 1.35% for the conventional once-through method and the proposed method, respectively. Thus remarkable improvement was achieved by the present method.

Once-through method



On-flight method



**Figure.8 Difference of k-effective and pin-power in the conventional method and the proposed method**

#### 4. CONCLUSIONS

A hybrid method of MOC and  $S_N$  nodal was developed to accurately calculate 3-D power distribution. Assembly calculations were performed based on MOC using the boundary condition calculated from the  $S_N$  nodal method. The core calculations were performed using the cell-averaged cross sections from the assembly calculations. Thus, the proposed method is called as an on-flight method.

To preserve reaction rates in each cell, the leakage dependent SPH method was used, and to calculate the cell averaged cross sections accurately when the neutron leakage becomes remarkable, an assembly model including the two cells of water reflector was used for the C5G7 benchmark. The proposed method has been applied to the 2-D and 3-D C5G7 benchmark problems. From the numerical results, it was found that the proposed method improved the accuracy compared to the conventional once-through method.

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