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DISCRETE ORDINATES ALBEDO BOUNDARY CONDITIONS FOR ONE-SPEED EIGENVALUE PROBLEMS IN X,Y GEOMETRY

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ABSTRACT

We describe in this paper approximate albedo boundary conditions for monoenergetic discrete ordinates (S_N) eigenvalue problems in X,Y geometry for criticality calculations. The albedo matrix substitutes approximately the reflector around the multiplying medium, as we neglect the transverse leakage terms within the reflector region, i.e., the reflector is assumed to be an infinite medium in the transverse direction. Although the present S_N albedo boundary conditions can be applied to numerous conventional S_N numerical methods for criticality calculations, we apply them to the recent hybrid spectral diamond-spectral Green's function-constant nodal (SD-SGF-CN) method. Numerical results to two typical model problems are shown to illustrate the method's accuracy.

1. INTRODUCTION

Non-multiplying regions around nuclear reactor cores are important as they reduce neutron leakage from the fuel regions (Duderstadt and Hamilton, 1976). However, since those regions such as moderator, reflector and structural materials do not generate power, we could improve the efficiency of discrete ordinates (S_N) codes for criticality calculations by eliminating the explicit numerical calculations within the non-multiplying regions around the active domain. This can be done by applying albedo boundary conditions, that approximately substitute the reflective properties of the non-active media around the core. *Albedo*, the latin word for "whiteness", was defined by Lambert as the fraction of the incident light reflected diffusely by a surface (Pannekoek, 1961). In this paper, we have extended the original concept of albedo to the diffuse reflection of neutrons.

Although the present S_N albedo boundary conditions can be applied to numerous conventional S_N numerical methods for criticality calculations, such as the linear diamond (DD) method (Lewis and Miller, 1993), or the classical nodal methods (Walters, 1986; Azmy, 1988), we apply them to the recent hybrid spectral diamond-spectral Green's function-constant nodal (SD-SGF-CN) method (Alves Filho *et al.*, 1999).

In deriving the S_N albedo matrix, we transverse-integrate the one-speed S_N equations in X,Y geometry inside the reflector region contiguous to the active boundary node of the spatial grid set up on the domain. That is, for the x direction, we integrate the

S_N equations inside the reflector region in the y direction, neglect the transverse leakage terms and solve the resulting homogeneous "one-dimensional" transverse-integrated S_N nodal equations in the x direction analytically by performing a spectral analysis (Barros *et al.*, 1999). The procedure follows two major steps: (i) the use of the familiar discretized spatial balance S_N equations (Lewis and Miller, 1993), with neglect of the leakage terms in the y direction, and (ii) the use of the non-standard spectral Green's function (SGF) auxiliary equations, that have parameters to preserve the analytical general solution of the homogeneous "one-dimensional" transverse integrated S_N nodal equations in the x direction. The procedure for the y direction follows similar steps. Therefore, by substituting the SGF auxiliary equations into the discretized spatial balance S_N equations, we can relate the neutron angular fluxes backscattered into the active node to the neutron angular fluxes entering the reflector from the active node, since vacuum boundary conditions apply on the outer boundaries of the reflector regions.

At this point, we remark that the only approximation that we consider in the derivation of the S_N albedo matrices for S_N eigenvalue problems in X,Y geometry is the neglect of the transverse leakage terms. Therefore, the S_N albedo matrices for S_N eigenvalue problems in slab geometry are "exact", except for the computational finite arithmetic (de Abreu and Barros, 1994). In case the approximate S_N albedo matrices introduce no significant errors to S_N criticality calculations in X,Y geometry, they should improve the efficiency of classical S_N computational codes, as they substitute approximately the non-multiplying regions around the active domain. Therefore, there is no need to perform explicit numerical calculations inside the reflector regions, for example. This positive feature is expected to be specially noticeable for fine grid S_N numerical methods, such as the DD method.

At this point, we present an outline of the remainder of this paper. In section 2, we present the mathematical preliminaries; in section 3, we describe how we determine the approximate S_N albedo matrices. In section 4 we show numerical results to two typical test problems and give a brief discussion with suggestions for future work.

2. MATHEMATICAL PRELIMINARIES

Let us consider the one-speed S_N equations in X,Y geometry with isotropic scaterring

$$\mu_m \frac{\partial}{\partial x} \psi_m(x,y) + \eta_m \frac{\partial}{\partial y} \psi_m(x,y) + \sigma_T \psi_m(x,y) = \sigma_S \sum_{n=1}^{M} \psi_m(x,y)\, w_n, \qquad (1)$$

$$m = 1 : M,\ M = N(N+2)/4 \ .$$

Here the notation is standard (Lewis and Miller, 1993) and Eq. (1) holds inside a homogeneous non-multiplying medium, e.g., the reflector region around a nuclear reactor core.

Now we consider a rectangular spatial grid Ω, where each node $\Omega_{i,j}$ has width h_i and height k_j, with i = 1 : (I +1) and j = 1 : (J +1). Viz Figure 1.

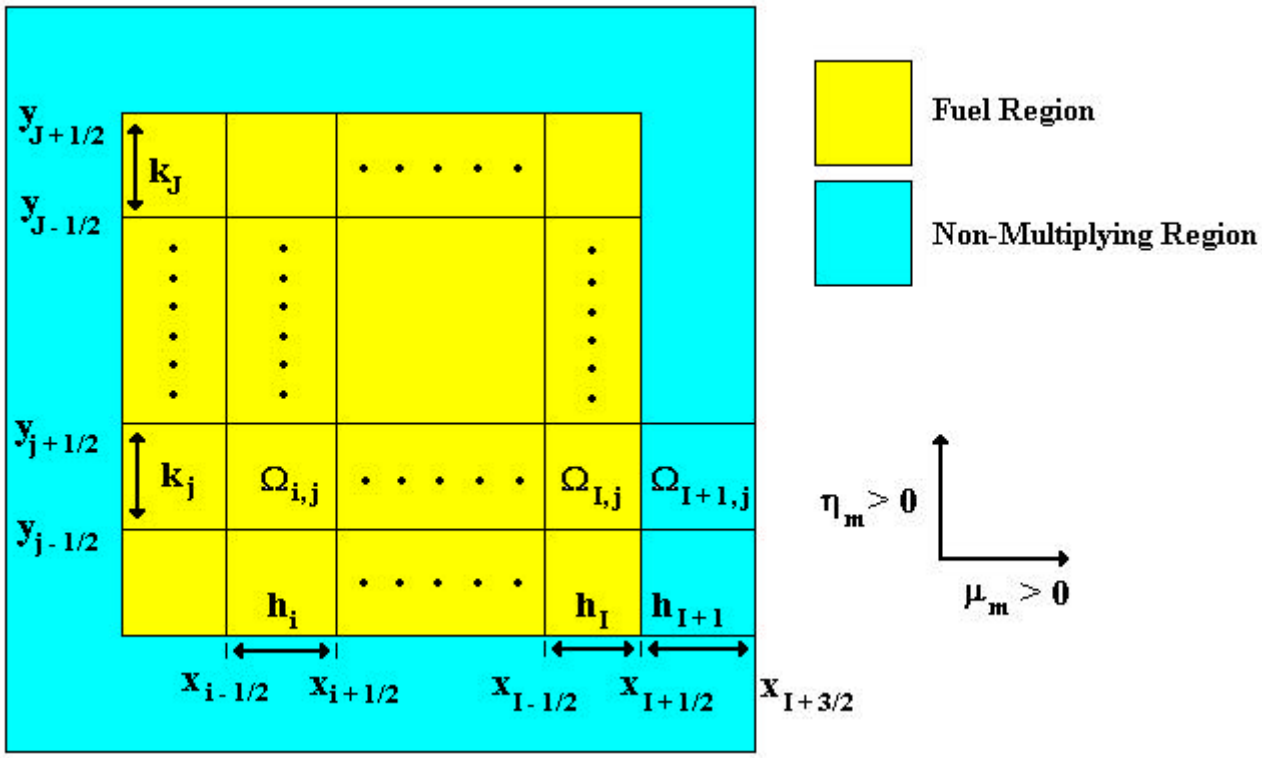


Figure 1. Spatial Grid Ω.

Further, we apply the operator

$$\frac{1}{k_j}\int_{y_{j-1/2}}^{y_{j+1/2}} (\,.\,)\, dy \tag{2}$$

in Eq. (1) within an arbitrary node $\Omega_{I+1,j}$ inside the reflector. The result is

$$\mu_m \frac{d}{dx}\tilde{\psi}_{m,j}(x) + \sigma_{T\,I+1,j}\,\tilde{\psi}_{m,j}(x) = \sigma_{S_{I+1,j}} \sum_{n=1}^{M} \tilde{\psi}_{n,j}(x)\, w_n - \frac{\eta_m}{k_j}\left[\psi_m(x, y_{j+1/2}) - \psi_m(x, y_{j-1/2})\right] \quad , \quad m = 1:M, \tag{3}$$

where $x \in \Omega_{I+1,j}$ and the total ($\sigma_{T\,I+1,j}$) and scattering ($\sigma_{S_{I+1,j}}$) cross sections are constant in node $\Omega_{I+1,j}$. Moreover $\tilde{\psi}_{m,j}(x)$ is the y direction node-edge average angular flux.

By neglecting the transverse leakage term in Eq. (3), i.e., by considering the reflector region as an infinite medium in the transverse direction (y direction in this case), we obtain the "one-dimensional" S_N equations

$$\mu_m \frac{d}{dx} \tilde{\psi}_{m,j}(x) + \sigma_{T\,I+1,j}\, \tilde{\psi}_{m,j}(x) = \sigma_{S\,I+1,j} \sum_{n=1}^{M} \tilde{\psi}_{n,j}(x)\, w_n \ , \qquad (4)$$

$$m = 1 : M \ , \ x \in \Omega_{I+1,\,j} \ .$$

In order to determine the analytical general solution of the Eq. (4), we perform a spectral analysis as described in (Barros *et al*., 1999). The result is

$$\tilde{\psi}_{m,j}(x) = \sum_{\ell=1}^{M} \alpha_\ell \; a_m^x \, (\vartheta_\ell) \exp\left(-\frac{\sigma_{T_{I+1,j}}\, x}{\vartheta_\ell}\right) \quad , m = 1 : M \quad , \qquad (5)$$

where α_ℓ are arbitrary constants and ϑ_ℓ are M real numbers that appear in $\pm$ pairs, due to the symmetry of conventional angular quadrature sets (Lewis and Miller, 1993).

At this point we remark that the only approximation considered here, is the transverse direction infinite medium approximation in Eq. (3). For the y direction, we proceed similary to obtain an equation in the y variable analogous to Eq. (5).

3. APPROXIMATE S_N ALBEDO

Let us integrate Eq. (1) inside an arbitrary node $\Omega_{I+1,\,j}$ within the reflector to obtain the familiar discretized spatial balance S_N equations

$$\frac{\mu_m}{h_{I+1}}\left[\tilde{\psi}_{m,j}(x_{I+3/2}) - \tilde{\psi}_{m,j}(x_{I+1/2})\right] + \frac{\eta_m}{k_j}\left[\hat{\psi}_{m,i}(y_{j+1/2}) - \hat{\psi}_{m,i}(y_{j-1/2})\right] +$$

$$\sigma_{T\,I+1,j}\, \overline{\psi}_{m,I+1,j} = \sigma_{S\,I+1,j} \sum_{n=1}^{M} \overline{\psi}_{n,I+1,j}\, w_n \ , \ m = 1 : M . \qquad (6)$$

Here $\hat{\psi}_{m,i}(y)$ is the x direction node-edge average angular flux, and $\overline{\psi}_{m,I+1,\,j}$ is the node-average angular flux. Furthermore, in order to determine the approximate S_N albedo for the x direction, we neglect the transverse leakage terms in the y direction in Eq. (6) to obtain the "one-dimensional" discretized spatial balance S_N equations

$$\frac{\mu_m}{h_{I+1}}\left[\tilde{\psi}_{m,j}(x_{I+3/2}) - \tilde{\psi}_{m,j}(x_{I+1/2})\right] + \sigma_{T\,I+1,j}\, \overline{\psi}_{m,I+1,j} =$$

$$\sigma_{S\,I+1,j} \sum_{n=1}^{M} \overline{\psi}_{n,I+1,j}\, w_n \ , \ m = 1 : M . \qquad (7)$$

Moreover, we consider the non-standard spectral Green's function (SGF) auxiliar equations

$$\overline{\psi}_{m,I+1,j} = \sum_{\mu_n > 0} \theta_{m,n} \tilde{\psi}_{n,j}(x_{I+1/2}) + \sum_{\mu_n < 0} \theta_{m,n} \tilde{\psi}_{n,j}(x_{I+3/2}) \ , \quad m = 1 : M \ , \tag{8}$$

where the parameters $\theta_{m,n}$ depend upon the nuclear properties and width of the reflector region, and they relate the node-average angular flux within the reflector in a fixed angular direction *m* to the node-edge average angular fluxes in all the incoming directions. To determine the parameters $\theta_{m,n}$ we substitute Eq. (5) into the SGF auxiliary equations (8), bearing in mind the average definitions. A detailed description of this procedure can be found in (Barros and Larsen, 1992).

Considering that vacuum boundary conditions apply on the outer boundaries of the reflector regions for criticality calculations, that is

$$\tilde{\psi}_{m,j}(x_{I+3/2}) = 0 \ , \ \mu_m < 0 \ , \tag{9}$$

viz Figure 1, we substitute the SGF auxiliary equation (8) into the "one-dimensional" spatial balance equation (7) to eliminate the node-average angular fluxes. Therefore, we are left with a system of M algebric linear equations in the y direction node-edge average angular fluxes *only*. After some algebra, we can write this system in the following matrix compact form

$$\tilde{\psi}_j^{\mu_m < 0}(x_{I+1/2}) = \underline{\underline{\Lambda}}_x^R \tilde{\psi}_j^{\mu_m > 0}(x_{I+1/2}) \tag{10}$$

where the M/2 x M/2 matrix $\underline{\underline{\Lambda}}_x^R$ is termed the approximate S_N albedo matrix to the right hand side boundary of the domain, viz Figure 1. The entries of this albedo matrix depend upon (i) the discrete ordinates angular quadrature set, (ii) the cross sections and width of the reflector region, and (iii) the parameters $\theta_{m,n}$ of SGF auxiliary equations. The M/2-dimensional vectors $\tilde{\psi}_j$ contain the y direction node-edge average angular fluxes at $x_{I+1/2}$ entering the reflector ($\mu_m > 0$) or entering the fuel region ($\mu_m < 0$). To obtain the albedo matrices for the left hand side boundary conditions, as well as for the top and bottom, we proceed similarly.

4. NUMERICAL RESULTS AND CONCLUDING REMARKS

In this secion we consider two test problems that we model using the level symmetric S_4 angular quadrature set (Lewis and Miller, 1993). Model problem No. 1 is represented in Figure 2 and the material data are given in Table 1. Table 2 lists the numerical results generated for the effective multiplication factor (k_{eff}) by the recent hybrid SD-SGF-CN method on various spatial grids with both explicit reflector and the offered approximated S_N albedo boundary conditions. As we see, the use of the present albedo boundary conditions does not increase significantly the relative deviations with respect to the fine grid DD results.

Table 1. Material data to Model Problem No.1.

Zone Number	σ_T	σ_S	$\nu\sigma_F$
1	2.22589E-1[a]	2.20563E-1	2.83283E-3
2	2.16566E-1	2.10697E-1	1.04347E-2
3	3.01439E-1	2.96069E-1	5.13036E-4
4	2.52250E-1	2.50794E-1	0.0

[a] Read as 2.22589×10^{-1}.

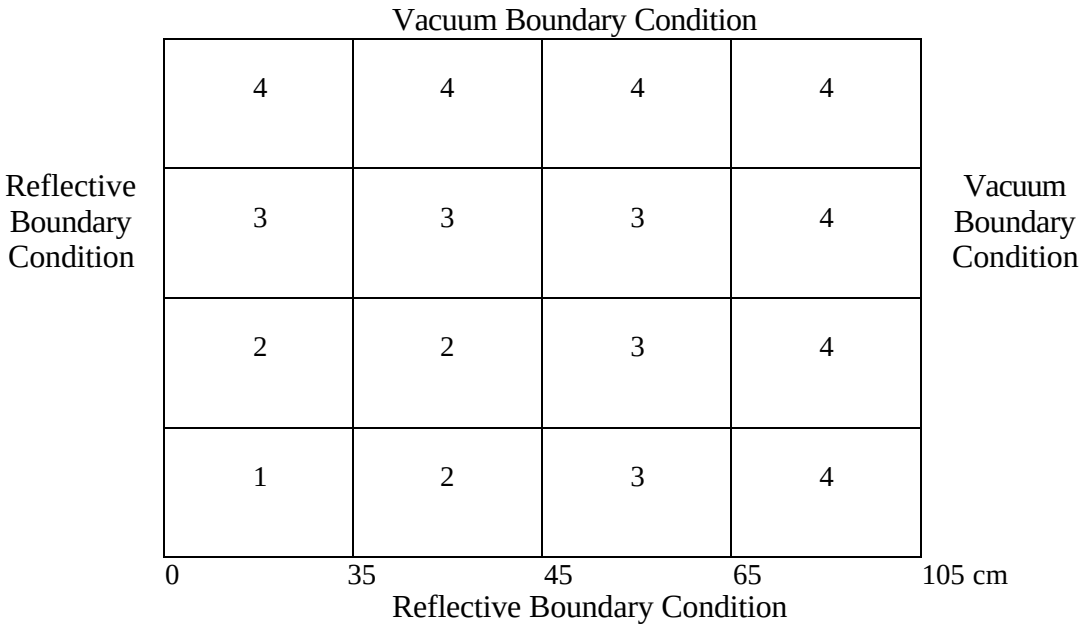


Figure 2. Model Problem No. 1.

Table 2. Numerical Results for Model Problem No. 1.

Spatial Grid Γ_n^a	Numerical Method	k_{eff}	Relative Deviation (%) [e]
Γ_2	SD-SGF-CN [b]	0.96865121	0.67
	SD-SGF-CN-ALB [c]	0.96901281	0.71
Γ_3	SD-SGF-CN	0.96395579	0.18
	SD-SGF-CN-ALB	0.96459353	0.25
Γ_4	SD-SGF-CN	0.96273334	0.06
	SD-SGF-CN-ALB	0.96340257	0.12
Γ_5	SD-SGF-CN	0.96235346	0.02
	SD-SGF-CN-ALB	0.96297753	0.08
Γ_6	SD-SGF-CN	0.96224372	0.00
	SD-SGF-CN-ALB	0.96280970	0.06
Γ_7	SD-SGF-CN	0.96221464	0.00
	SD-SGF-CN-ALB	0.96273284	0.06
Γ_8	DD [d]	0.96220092	

[a] $2^n / 4$ spatial nodes per region in each spatial direction.

[b] *Spectral diamond-spectral Green's function-constant nodal* method with explicit reflector.

[c] *Spectral diamond-spectral Green's function-constant nodal* method with albedo boundary conditions.

[d] *Diamond difference* method.

[e] Relative deviation with respect to the DD fine-mesh solution.

Moreover, Figure 3 displays the power density (Watt / cm^3) distribution as generated by the SD-SGF-CN method on a spatial grid composed of one node per region, assuming unit total power density generation.

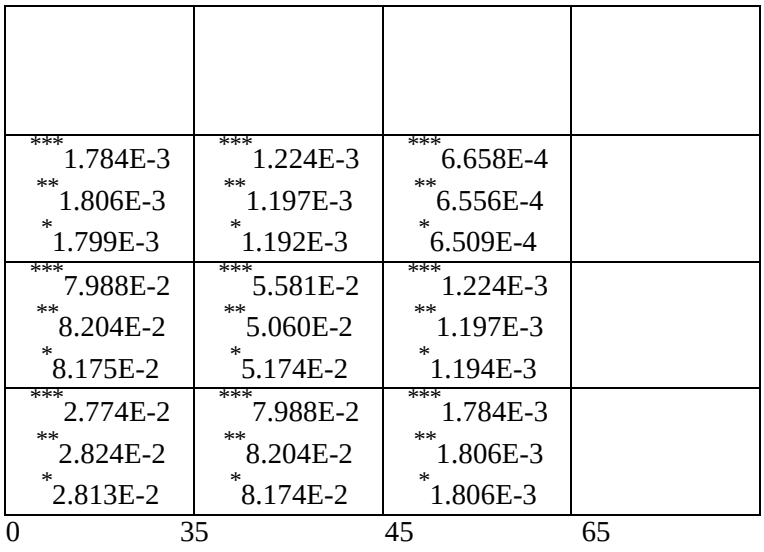


Figure 3. Power Density Distribution in Model Problem No. 1.

As we see, the power density distribution as generated by the SD-SGF-CN method on a very coarse spatial grid with explicit reflector and using albedo boundary conditions, did not deviate significantly from the DD fine grid results..

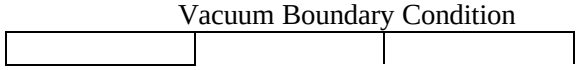
Our second model problem consists of a heterogeneous critical system, composed of three different material zones, viz Figure 4. Table 3 gives the material data for the three zones: two active zones (Pu – 239) and one reflector (water) around the core (Sood *et al.*, 1999).

Table 3. Material data to Model Problem No. 2.

Zone Number	σ_T	σ_S	$\nu\sigma_F$
1	3.26400E-1[a]	2.25216E-1	0.26438
2	3.26400E-1	2.25216E-1	0.27174
3	3.26400E-1	2.93760E-1	0.0

[a] Read as 3.26400×10^{-1}.

The hybrid SD-SGF-CN method generated k_{eff} = 1.0038254 with explicit reflector, and k_{eff} = 1.0039249 with albedo boundary conditions on a coarse spatial grid composed of one node per region. These results are within reasonable deviations from the DD fine grid result k_{eff} = 0.9999487. Moreover, Figure 5 shows the accurate numerical results generated for the power density distribution by the SD-SGF-CN method with explicit reflector and using the albedo boundary conditions on a spatial grid composed of one node per region, again assuming total power density generation equal to 1 Watt/cm^3.



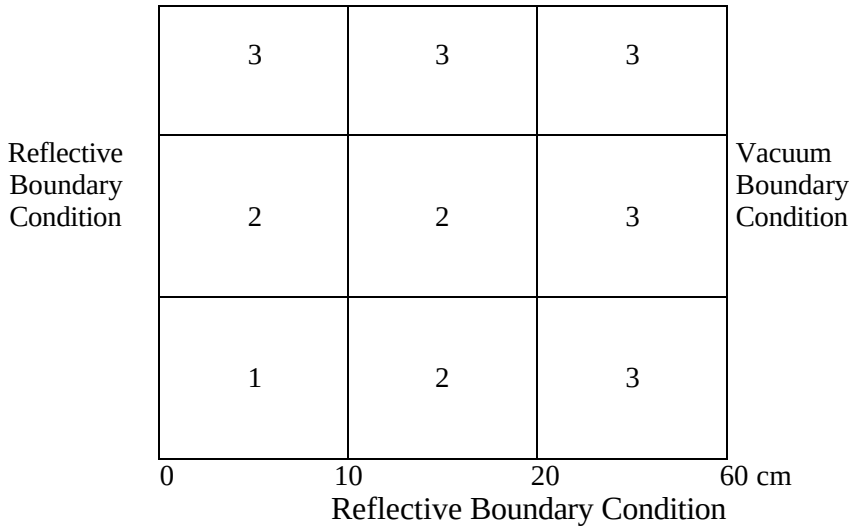


Figure 4. Model Problem No. 2 (critical system, k_{eff} = 1.0).

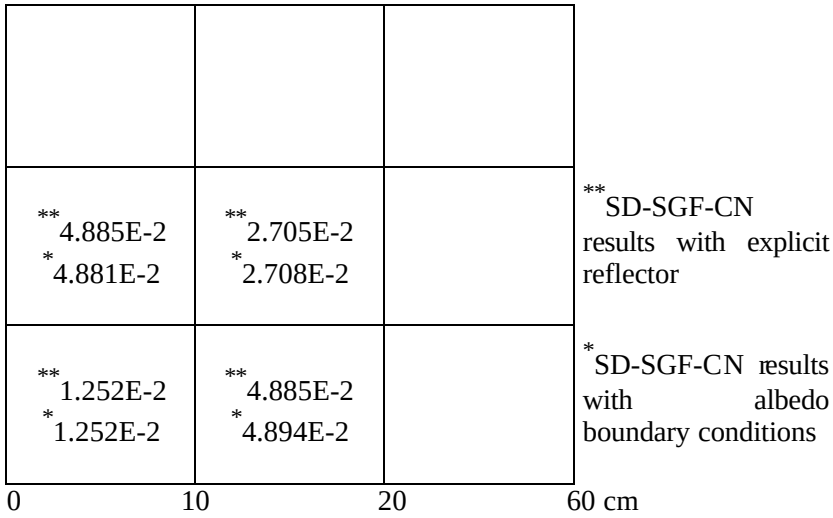


Figure 5. Power Density Distribution in Model Problem No. 2.

Based on the numerical results presented in this section, we list a number of concluding remarks and suggestions for future work:

- the approximate S_N albedo boundary conditions for criticality calculations substitutes very accurately the reflector around the active core;
- in applying the approximate S_N albedo boundary conditions in the x and y directions, the symmetric distribution of the numerical results is slightly perturbed, viz Figures 3 and 5. We are investigating this non-physical characteristic, that we believe is related to finite arithmetic computations;
- as future work, our next step is to determine approximate S_N albedo matrices for multilayer non-multiplying regions around the active core, e.g., baffle-reflector system;

- for practical applications in nuclear reactor global calculations, the multigroup approximate S_N albedo boundary conditions are of great interest to account for the neutron energy change in nuclear interactions.

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REFERENCES

1 Alves Filho, H., Barros, R.C., Carvalho, F.C., 1999. The Hybrid Spectral Diamond-Spectral Green's Function-Constant Nodal Method for One-Speed X,Y-Geometry S_N Eigenvalue Problems, *Proceedings of the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analyses*, Vol. 2, Madri, pp. 1608-1617.

2. Azmy, Y.Y., 1988, The Weighted Diamond-Difference Form of Nodal Transport Methods, *Nucl. Sci. Eng.*, **98**, 29-40.

3. Barros, R.C., Alves Filho, H., Carvalho, F.C., 1999. Recent Advances in Spectral Nodal Methods for X,Y-Geometry Discrete Ordinates Deep Penetration and Eigenvalue Problems. *Prog. Nucl. Energy.*, **35**, 293-331.

4. Barros, R.C., Larsen, E.W., 1992. A Spectral Nodal Method for One-Group X, Y-Geometry Discrete Ordinates Problems. *Nucl. Sci. Eng.*, **111**, 34-45.

5. de Abreu, M.P., Barros, R.C., 1994. Um Esquema para Reconstrução Analítica da Solução Dominante de Problemas de Autovalor Unidimensionais Multigrupo na Formulação de Ordenadas Discretas, Anais do XVII Congresso Nacional de Matemática Aplicada e Computacional. Vol. I, Vitória, pp. 256-260.

6. Duderstadt, J.J., Hamilton, L.J., 1976. *Nuclear Reactor Analysis*, John Wiley & Sons, New York.

7. Lewis, E.E., Miller, W.F.Jr., 1993. *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, Ilinois.

8. Pannekoek, A., 1961, *A History of Astronomy*, Rover Publications, Inc., New York.

9. Sood, A., Forster, R. A, Parsons, D.K. Analytical Benchmark Test Set for Criticality Code Verification, LA-13511, 1999.

10. Walters., W.F., 1986. The Relation Between Finite Element Methods and Nodal Methods in Transport Theory, *Prog. Nucl. Energy*, **18**, 21-26.