M&C 2001 Salt Lake City, Utah, USA, September 2001.

INTRA-NODAL REACTIVITY CALCULATIONS BASED ON THE VARIATIONAL NODAL METHOD

A. Rineiski
Institute for Nuclear and Energy Technologies
IKET, Forschungszentrum Karlsruhe
Hermann-von-Helmholtz-Platz 1
D-76344 Eggenstein-Leopoldshafen, Germany
E-mail: Andrei.Rineiski@iket.fzk.de

Keywords: Neutron Transport, Variational Nodal Method, Perturbation Theory, Intra-nodal Reactivity Worths

ABSTRACT

The Variational Nodal Method is an efficient tool for determining the neutron transport in reactor analyses. The (inner) iterative scheme employs response matrices computed for homogeneous nodes from precalculated large arrays of integrals over trial and basis functions. It was demonstrated that for heterogeneous nodes, these arrays can be computed by numerical integration. In the paper a technique is presented that allows to avoid numerical integration (while computing "heterogeneous" response matrices) for some important cases. One can also apply this technique for computing contributions from parts of the nodes to the reactivity integrals; this feature can be useful for providing spatial reactivity distributions for thermal-hydraulics models which may require a significantly finer spatial mesh compared to the original neutronics nodal model.

1. INTRODUCTION

The Variational Nodal Method (VNM) is implemented in the VARIANT code (Lewis, 1996) and provides opportunities for solving the neutron transport and diffusion equations in various 3-D geometries.

In the VNM solution scheme, integrals of the following types (from Eq. (1), it is evident that the method cannot be applied when vacuum nodes are contained within the reactor) must be calculated for each group and node (group and node indices are omitted hereafter):

$$A'_{t,i,j} = \int_V \int \sigma_t^{-1}(r)(\Omega\nabla f_i(\Omega,r))(\Omega\nabla f_j(\Omega,r))d\Omega dV\,, \tag{1}$$

$$A_{t,i,j} = \int_V \int \sigma_t(r)\, f_i(\Omega,r) f_j(\Omega,r) d\Omega dV\,, \tag{2}$$

$$A_{x,i,j} = \int_V \sigma_x(r) f_i(r) f_j(r) dV , \tag{3}$$

where

$$f_i(r) = \int f_i(\Omega, r) d\Omega , \tag{4}$$

V is the volume of the node, $\sigma_t(r)$ is the total cross-section, $\sigma_x(r)$ is a partial cross-section for reaction x (removal, scattering, ...), $f_i(\Omega, r)$, (i=1,...I) are orthonormal basis functions depending on space position *r* and angle Ω:

$$\frac{1}{V} \int_V \int f_i(\Omega, r) f_j(\Omega, r) d\Omega dV = \delta_{i,j} . \tag{5}$$

These basis functions are used to approximate the (real or adjoint) even-parity flux in angle and space (within each node):

$$\psi(\Omega, r) = \sum_{i=1}^{I} \zeta_i f_i(r, \Omega) . \tag{6}$$

A similar approximation is used for the source term (assuming isotropic source and scattering).

The functions $f_i(\Omega, r)$ are products of the known spatial and angular functions representing the first few members of classical complete orthonormal sets of mathematical functions: the spatial functions are constructed from Legendre polynomials, the angular functions are spherical harmonics. ζ_i are the expansion coefficients (to be determined for each group and node when VARIANT solves the transport equation), the expansion orders in space and in angle being defined by the user. These orders determine the number of basis functions in space (I_s), and in angle (I_a), the total number of the basis functions being $I = I_s I_a$. These basis functions are ordered in such a way that the first I_s functions are the spatial basis functions, thus the first I_s expansion coefficients ζ_i define the scalar flux:

$$\phi(r) = \sum_{i=1}^{I_s} \zeta_i f_i(r) . \tag{7}$$

When the nodes are homogeneous, the integrals (1), (2), (3) are calculated analytically. The values defined by Eqs. (2), (3) are computed easily (by taking into account orthonormality of the basis functions within each node). The values defined by Eq. (1) are obtained from matrices precalculated in similar geometry for the 'unity' node (with volume of 1 cm^3) by employing simple transformations involving a change of variables. These matrices (for the 'unity' node) can be precalculated once, they are included currently as data statements in the Fortran source of VARIANT.

If one has to calculate integrals (1), (2), (3) for heterogeneous nodes, more complex calculations are required. For 2-D XY heterogeneous geometry models, it was proposed (Fanning, 1997) to compute these integrals numerically (in space), Gaussian quadratures being used. It was shown that for these heterogeneous models, direct taking into account of intra-nodal cross-section spatial dependence may provide better results than smearing of cross-sections within nodes, these smeared cross-sections then being used for VNM calculations (hereafter we do not discuss how to prepare the effective cross-sections for heterogeneous nodes).

Direct numerical integration makes the computations more complicated and time-consuming. In this paper, it will be shown how to avoid numerical integration for some simple cases. The results, however, may be generalized for more complicated models.

2. ANALYTICAL CALCULATION OF MATRICES A FOR AXIALLY HETEROGENEOUS NODES

Let us consider a 3D (HEX-Z or X-Y-Z) reactor model in which some nodes are heterogeneous in axial direction (only in axial). We will suppose that the node is subdivided into N axial parts, within each part (z_k, z_{k+1}), k=1, 2, ... N, the cross-sections being homogeneous. This may be, for example, a node which includes the bottom of a movable control rod, a lower part of this node being assigned to the control rod follower. Then integrals in (1), (2), (3) may be calculated as

$$A'_{t,i,j} = \sum_{k=1}^{N} \sigma_{t,k}^{-1}(r) \int_{V_k} \int (\Omega \nabla f_i(\Omega, r))(\Omega \nabla f_j(\Omega, r)) d\Omega dV \,, \tag{8}$$

$$A_{t,i,j} = \sum_{k=1}^{N} \sigma_{t,k}(r) \int_{V_k} \int f_i(\Omega, r) f_j(\Omega, r) d\Omega dV \,, \tag{9}$$

$$A_{x,i,j} = \sum_{k=1}^{N} \sigma_{x,k}(r) \int_{V_k} f_i(r) f_j(r) dV \,, \tag{10}$$

Within each k-th sub-node, the functions $f_i(\Omega, r)$ are no longer orthonormal. Let us introduce suitable functions $f_{k,i}(\Omega, r)$ which would be orthonormal there. Assuming that both $f_{k,i}(\Omega, r)$ and $f_i(\Omega, r)$ are constructed from the same set of spatial and angular polynomials, one can expand $f_i(\Omega, r)$ within each sub-node *k* as

$$f_i(\Omega, r) = \sum_{m=1}^{I} C_{k,m,i} f_{k,m}(\Omega, r) \,, \tag{11}$$

where $f_{k,i}(\Omega, r)$ are orthonormal within the sub-node:

$$\frac{1}{V_k}\int\int_{V_k} f_{k,i}(\Omega,r) f_{k,j}(\Omega,r) d\Omega dV = \delta_{i,j} . \quad (12)$$

Then

$$C_{k,m,i} = \frac{1}{V_k}\int\int_{V_k} f_i(\Omega,r) f_m(\Omega,r) d\Omega dV . \quad (13)$$

Employing Eq. (11), one can transform Eqs. (8)

$$A'_{t,i,j} = \sum_{k=1}^{N}\sum_{m=1}^{I}\sum_{l=1}^{I} C_{k,m,i} C_{k,l.j} A'_{t,k,m,l} , \quad (14)$$

where

$$A'_{t,k,i,j} = \sigma_{t,k}^{-1}(r)\int\int_{V_k} (\Omega\nabla f_{k,i}(\Omega,r))(\Omega\nabla f_{k,j}(\Omega,r)) d\Omega dV . \quad (15)$$

Eqs. (9), (10) can be transformed in the same manner. The values defined by Eq. (15) (as well as the corresponding integrals related to Eqs. (9), (10)) may be computed in the usual way (for each sub-node as for a conventional homogeneous node). Therefore, knowing the matrices C, one can obtain the matrices A (for axially heterogeneous nodes) by simple summation, thus avoiding any numerical integration. The application of this method is justified when the flux in a heterogeneous node can be sufficiently accurately approximated in space by the few first basis functions because otherwise it might be better to deal with finer nodes.

3. CALCULATION OF THE MATRIX C FOR A PARTICULAR LAYER

In VARIANT, the following products are used as basis functions:

$$f_i(\Omega,x,y,z) = g_i(\Omega) W_i(x,y) Z_i(z), \quad (16)$$

The axial basis functions are

$$Z_i(z) = \sqrt{(2l(i)+1)} P_{l(i)}\left(\frac{2z - z_N - z_1}{z_N - z_1}\right), \quad (17)$$

where $P_{l(i)}$ are Legendre polynomials of order l(i), the integer function l(i) is defined by the ordering of the basis functions, z_N and z_1 are the lower and upper node boundary positions, respectively.

Let us define functions

$$f_{k,i}(\Omega,x,y,z) = g_i(\Omega) W_i(x,y) Z_{k,i}(z), \quad (18)$$

where

$$Z_{k,i}(z) = \sqrt{(2l(i)+1)}P_{l(i)}(\frac{2z - z_{k+1} - z_k}{z_{k+1} - z_k}), \tag{19}$$

Then

$$C_{k,m,i} = G_{m,i} D_{m,i} E_{k,l(m).l(i)}, \tag{20}$$

where

$$G_{m,i} = \int g_i(\Omega) g_m(\Omega) d\Omega, \tag{21}$$

$$D_{m,i} = \frac{z_{k+1} - z_k}{V_k} \int W_i(x,y) W_m(x,y) dxdy, \tag{22}$$

$$E_{k,m,i} = \frac{\sqrt{(2m+1)(2i+1)}}{z_{k+1} - z_k} \int_{z_k}^{z_{k+1}} P_m(\frac{2z - z_{k+1} - z_k}{z_{k+1} - z_k}) P_i(\frac{2z - z_N - z_1}{z_N - z_1}) dz. \tag{23}$$

The matrix *G* consists of zero and unity entries (because the angular basis functions are orthonormal) and may be defined easily once one knows the ordering of the basis functions. In rectangular geometry, the functions $W_i(x,y)$ are also orthonormal, therefore, the matrix *D* has also only zero and unity entries. For hexagonal geometry, not all functions $W_i(x,y)$ are orthonormal, and the structure of the matrix *D* is a little bit more complicated (compared to rectangular geometry), but its few entries, which are not equal to zero and not equal to unity, may also precalculated only once.

Eq. (23) may be rewritten as

$$E_{k,m,i} = \sqrt{\frac{2i+1}{2m+1}} F_{k,m,i}, \tag{24}$$

where

$$F_{k,m,i} = \frac{2m+1}{2} \int_{-1}^{1} P_m(u) P_i(u\Delta u_k - \bar{u}_k) du, \tag{25}$$

$$\bar{u}_k = \frac{z_N + z_1 - 2z_k}{z_N - z_1}, \tag{26}$$

$$\Delta u_k = \frac{z_{k+1} - z_k}{z_N - z_1}. \tag{27}$$

Taking into account that the values defined by Eq. (25) are equal to zero for $m>i$ (a Legendre polynomial is orthogonal to any polynomial of lower order), one may calculate these values by employing the following recurrence formulae (Rineiski, 1989):

$$F_{k,0,0} = 1, \tag{28}$$

$$F_{k,0,1} = -\bar{u}_k, \tag{29}$$

$$F_{k,1,1} = \Delta u_k, \tag{30}$$

$$F_{k,m,i+1} = \frac{2i+1}{i+1}\left\{\frac{(m+1)\Delta u_k}{2m+3}F_{k,m+1,i} - \bar{u}_k F_{k,m,i} + \frac{m\Delta u_k}{2m-1}F_{k,m-1,i} - \frac{i}{2i+1}F_{k,m,i-1}\right\}. \tag{31}$$

In Eq. (31), the third term in the brackets is equal to zero for m=0.

4. INTRA-NODAL POWER DENSITY AND REACTIVITY WORTHS

Let us consider a problem when one has to calculate the power density and reactivity worths for small sub-nodes (in the axial direction) of rather big nodes (employed for spatial discretization in the VNM solution scheme). Hereafter, we will suppose that the even-parity real/adjoint flux expansion coefficients (for the VNM nodes) have already been obtained. It is no longer relevant whether the cross-sections have been preliminary smeared or the (potentially) more accurate integration technique (described in the previous section) was employed in the VNM solution scheme.

The power density in a sub-node is defined as:

$$p_k = V_k^{-1}\sigma_{power,k}\int\int_{V_k}\psi(\Omega,r))d\Omega dV, \tag{32}$$

and may be calculated employing Eqs. (6), (11) as:

$$p_k = \sigma_{power,k}\sum_{i=1}^{I_s} C_{k,1,i}\zeta_i. \tag{33}$$

This leads us to the idea of defining sub-node expansion coefficients as:

$$\zeta_{k,m} = \sum_{i=1}^{I} C_{k,m,i}\zeta_i. \tag{34}$$

For perturbation theory calculations with VNM (Laurin-Kovitz, 1995), the interface partial current moments are not needed (unlike in some other nodal methods). The perturbation theory integrals for entirely homogeneous nodes can be computed in two steps. During the first step, the scalar (inner) products of the real and adjoint flux moments are computed from the expansion coefficients. During the second step, the

integrals (reactivity effect contributions, β_{eff}, Λ, etc.) are computed from the scalar products and nuclear data (the nodal-wise cross-sections, delayed neutron data, velocities, etc.). The scalar products are of the following types:

$$< \Omega\nabla\psi, \Omega\nabla\psi^* >= \sum_{i=1}^{I}\sum_{j=1}^{I} \zeta_i B_{i,j} \zeta_j^*, \tag{35}$$

$$< \psi, \psi^* >= V \sum_{i=1}^{I} \zeta_i \zeta_j^*, \tag{36}$$

where

$$B_{i,j} = \int_V \int (\Omega\nabla f_i(\Omega, r))(\Omega\nabla f_j(\Omega, r)) d\Omega dV \ . \tag{37}$$

These scalar products can be used easily to compute reactivity worths related to entire nodes: the nodal cross-sections are just multiplied by these scalar products and then the products are summed in a certain way.

To retain this two-step scheme for the intra-nodal reactivity worth calculations, we will calculate the sub-node scalar products as:

$$< \Omega\nabla\psi, \Omega\nabla\psi^* >_k = \sum_{i=1}^{I}\sum_{j=1}^{I} \zeta_{k,i} B_{k,i,j} \zeta_{k,j}^*, \tag{38}$$

$$< \psi, \psi^* >_k = V \sum_{i=1}^{I} \zeta_{k,i} \zeta_{k,j}^*, \tag{39}$$

where

$$B_{k,i,j} = \int_V \int (\Omega\nabla f_{k,i}(\Omega, r))(\Omega\nabla f_{k,j}(\Omega, r)) d\Omega dV \ . \tag{40}$$

The integrals defined by Eq. (40) for sub-nodes may be computed in the same way as it is currently performed for entire (homogeneous) nodes.

5. NUMERICAL RESULTS

The proposed technique for the intra-nodal power density and reactivity worth curves computations was implemented into KIN3D, a kinetics and perturbation theory extension (Rineiski, 1997) for VARIANT, to provide neutronic parameters for an accident analysis code.

To test the new option, the calculations of the nodal/sub-nodal contributions to the reactivity effects related to control rod movement were performed for the Takeda 1 and Takeda 4 benchmark models (Takeda, 1991). In order to illustrate the type of these models, the horizontal cross-sections of the layouts are given in Fig. 1 and Fig. 2.

The Takeda 1 model is a thermal reactor; the core height is 30 cm; two axial reflectors (of 10 cm thick) are above and below the core. An important characteristic of this model is that the diffusion theory predicts the wrong sign of the control rod worth value. The Takeda 4 model is a fast system; the core height is 60 cm, two axial blankets (of 20 cm thick) and two axial reflectors (of 45 cm thick) are above and below the core.

These contributions were computed in three ways: (1) for a 'coarse' axial mesh, the contributions were evenly distributed to a finer axial mesh; (2) for the same coarse mesh, but then the flux/adjoint flux moments were 'remapped' to a finer axial mesh; (3) directly for the 'fine' mesh.

The results for the model 1 are presented in Table 1. The calculations were performed in X-Y-Z geometry with P_3 angular approximation and spatial approximation of the 4-th order. The coarse mesh size was 10 cm, the fine mesh size was 2.5 cm.

In Fig. 3 the results of Table 1 are presented in graphical form in the axial range 0 – 25 cm (1/2 core). These results show that the described method of calculations provides reasonable sub-nodal reactivity values (which certainly do not exactly agree with the figures provided in the 'fine' mesh case) and preserves the 'coarse' nodal reactivities.

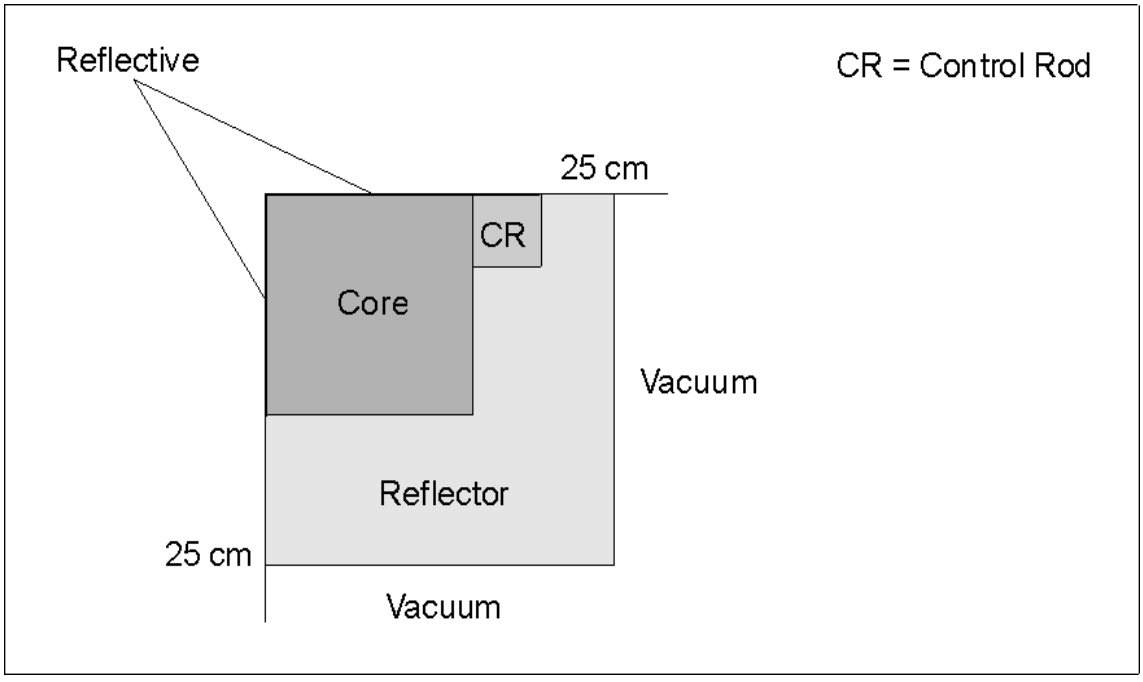

Fig. 1 Horizontal cross-sections of the Takeda 1 model in axial mid-plane

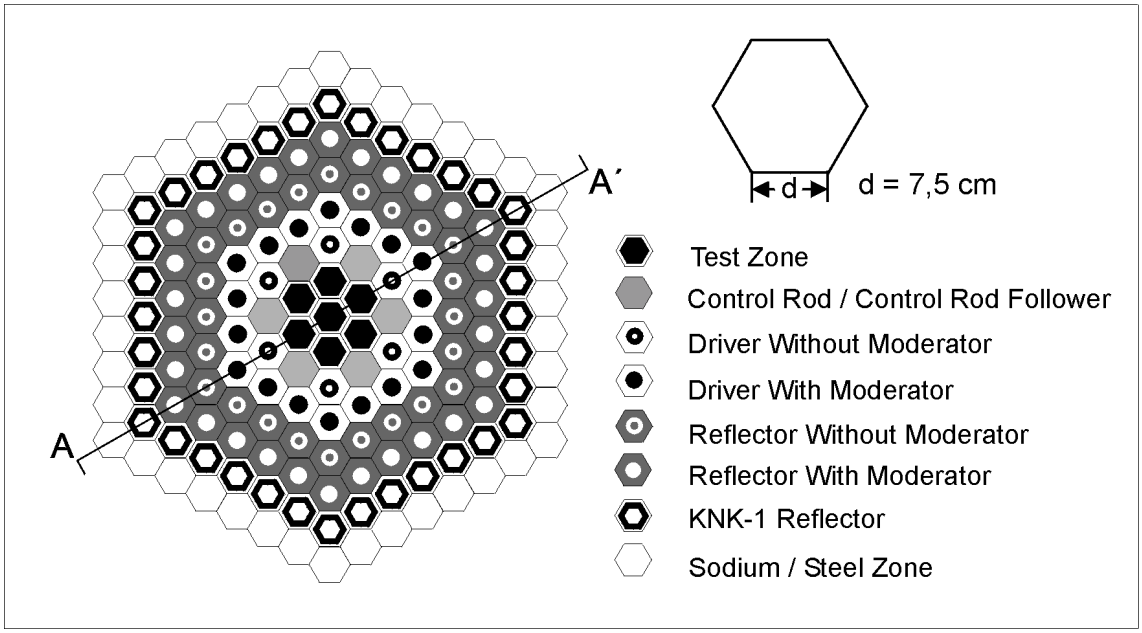

Fig. 2 Horizontal cross-sections of the Takeda 4 model in axial mid-plane

Table 1 Nodal (coarse, fine) and sub-nodal (evenly distributed, remapped) contributions to full control rod withdrawal effect for the Takeda 1 model

Axial position			Contributions to reactivity (pcm)		
	z_l (cm)	z_h (*cm*)	Coarse	Remapped	Fine
Blanket	0	2.5	-4.0	-5.6	-4.2
	2.5	5	-4.0	-8.5	-7.2
	5	7.5	-4.0	-5.9	-6.4
	7.5	10	-4.0	8.0	8.2
Total in Blanket	0	10	-12.0	-12.0	-9.5
1st Core node	10	12.5	81.2	38.4	41.3
	12.5	15	81.2	70.1	73.0
	15	17.5	81.2	99.1	99.9
	17.5	20	81.2	121.4	122.1
Total in 1st Core node	10	20	328.9	328.9	336.2
2nd Core node	20	22.5	141.1	136.5	138.3
	22.5	25	141.1	145.7	146.8
	25	27.5	141.1	145.7	146.8
	27.5	30	141.1	136.5	138.3
Total in 2nd Core node	20	30	564.4	564.4	570.2
Total in Reactor	0	50	1198.3	1198.3	1223.6

In Fig. 4 similar results are presented for the Takeda 4 model. The calculations were performed in HEX-Z geometry with of P_3 angular approximation and spatial approximation of the 4-th order. As in the previous case, good agreement between "remapped" and "fine" curves is demonstrated.

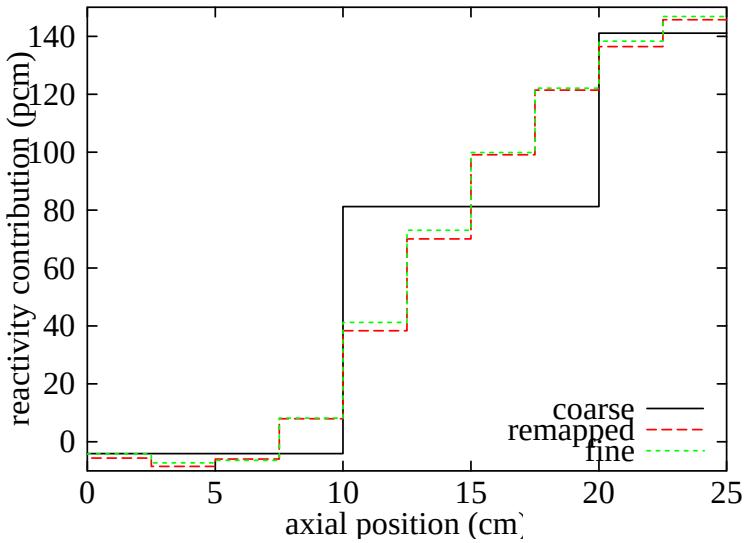

Fig. 3 Reactivity contributions to control rod withdrawal for the Takeda 1 model.

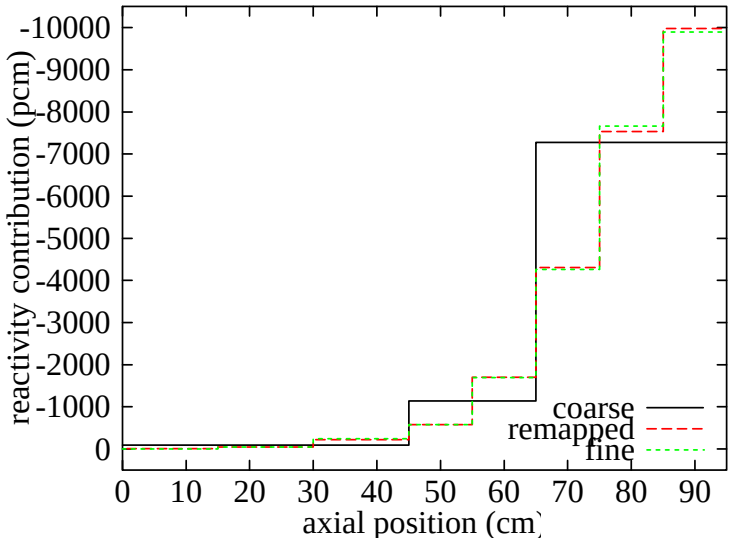

Fig. 4 Reactivity contribution to all control rods insertion for the Takeda 4 model.

The presented results show, that the fine spatial reactivity distributions can be determined with reasonable accuracy for coarse mesh models by employing the additional information about the flux and adjoint intra-nodal distributions. The computing time usually increases linearly (or faster) with increasing the number of nodes. That is why employing intra-nodal reactivity calculations with "coarse" direct and adjoint fluxes may

save computer time compared to direct “fine” flux and reactivity calculations (e.g. by a factor of 2 if the number of “fine” nodes is twice as the number of coarse nodes).

6. CONCLUSIONS

The proposed technique can be used to extend the existing VARIANT capabilities for flux calculations with axially heterogeneous nodes. It was tested in sub-nodal (in the axial dimension) reactivity worth calculations and provides reasonable results. This technique was used in creating an interface with a thermal hydraulics code, needing more detailed local information deduced from a proper specification of the material management not taken into account in the more crude calculation model applied for the overall real/adjoint flux calculations.

ACKNOWLEDGMENTS

The author thanks Dr. E. Kiefhaber for useful suggestions and comments.

REFERENCES

Fanning, T.H., Palmiotti, G., 1997. Variational Nodal Transport Method with Heterogeneous Nodes. *Nucl. Sci. Eng.* **127**, 154

Laurin-Kovitz, K.F., Lewis, E.E., 1995. Perturbation Theory Based on the Variational Nodal Transport Method in X-Y-Z Geometry. Proc. Int. Conf. on Mathematics and Computations, Reactor Physics and Environmental Analyses, Portland, Oregon, p. 970

Lewis, E.E., Carrico, C.B., Palmiotti, G., 1996. Variational Nodal Formulation for the Spherical Harmonics Equations. *Nucl. Sci. Eng.* **122**, 194

Rineiski, A., 1989. On the evaluation of group-to-group transfer cross-sections angular dependence. USSR Problems of Atom. Sci. Techn. (VANT), Series: Nuclear Constants, vol. 1, p. 81.

Rineiski, A., Doriath J.Y., 1997. Time-Dependent Neutron Transport with Variational Nodal Method, Proc. Joint Int. Conf. on Math. Methods and Supercomputing for Nuclear Applications, Saratoga Springs, New York, p. 1661

Takeda, T. et al., 1991. 3-D Neutron Transport Benchmarks, NEARCP-L-330, OECD/NEA report.