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A PRACTICAL IMPLEMENTATION OF A HIGHER ORDER TRANSVERSE LEAKAGE APPROXIMATION

Rian H. Prinsloo*and Djordje I Tomašević
Necsa
PO Box 582, Pretoria, 0001, South Africa
rian.prinsloo@necsa.co.za; djordje.tomasevic@necsa.co.za

ABSTRACT

Transverse integrated nodal diffusion methods currently represent the standard in full core neutronic simulation. The primary shortcoming in this approach, be it via the Analytic Nodal Method or Nodal Expansion Method, is the utilization of the quadratic transverse leakage approximation. This approach, although proven to work well for typical LWR problems, is not consistent with the formulation of nodal methods and can cause accuracy and convergence problems. In this work an improved, consistent quadratic leakage approximation is formulated, which derives from the class of higher order nodal methods developed some years ago. In this new approach, only information relevant to describing the transverse leakage terms in the zero-order nodal equations are obtained from the higher order formalism. The method yields accuracy comparable to full higher order methods, but does not suffer from the same computational burden which these methods typically incur.

Key Words: nodal diffusion methods, transverse leakage approximation, higher order methods

1. INTRODUCTION

The class of nodal diffusion methods [1–3], as applied to global reactor calculations [4–6], has grown into a mature and trusted technique in recent times. These coarse mesh methods provide substantial performance increases, while simultaneously maintaining high levels of accuracy. Coupled with appropriate homogenization techniques, and the generation of equivalence parameters [7], nodal methods have gained much favour in the power reactor industry, and mostly share three characteristics [8]:

1. Unknowns are defined in terms of volume-averaged fluxes and surface-averaged net or partial currents.
2. The volume (node) averaged fluxes and surface-averaged currents are related through auxiliary relationships. Such relationships, in the case of modern nodal methods, are often obtained via a transverse integration procedure.
3. Transverse leakage terms appear due to the transverse integration procedure, and these are approximated in some way. Typical approaches would include the "flat leakage" approximation, and the "quadratic leakage" approximation. The latter introduces a three

*Corresponding author

node quadratic fit for the transverse leakage term in the transversely integrated equations and has become the industry standard in Cartesian geometry.

Beyond these similarities, methods differ largely in the form of the intra-node solution. Two classes of methods, which are most often utilized, are the Analytic Nodal Method (ANM), and the polynomial method. In the case of the analytic method, the intra-node flux shape is the analytic solution of the one-dimensional transversely integrated diffusion equation. This approach requires no approximations other than the transverse leakage approximation mentioned in point three above. In one dimension, therefore, the analytic method is formally exact. A full description concerning the Analytic Nodal Method may be found in [2].

In the case of polynomial methods, the intra-node one-dimensional flux is approximated to the n^{th} order on some set of polynomial basis functions. Expansion coefficients may be determined in various ways, and the transverse leakage approximation is, of course, still required. Further details concerning the most widely used polynomial method, namely the Nodal Expansion Method (NEM), may be found in [3].

The pros and cons of these methods do not lead to any clear preference in selection, but some arguments [8] suggest that the ANM does exhibit both slight performance and accuracy advantages over its polynomial counterpart. Other classes of nodal methods, which do not require transverse integration, also exist and may be solved via various approaches such as direct polynomial expansion [9], analytic function expansion [11, 12], response matrix formalism [10] and plane wave approximation [13]. These approaches provide improved accuracy, but due to dense spatial coupling and large numbers of unknowns per calculational mesh, they may suffer from long and sometimes impractical running times.

In both the ANM and NEM approaches, which constitute the most widely used nodal approaches, the quadratic transverse leakage approximation is the major source of inaccuracy, but also of convergence problems. The standard method for generating the three leakage coefficients in a given direction is to apply a three-node quadratic fit of average transverse leakages in adjacent nodes. This approach uses information from the direction under consideration to construct the leakage shape from the transverse directions. This implies a certain level of long range coupling to betwen nodes and the statement regarding the quadratic transverse leakage approximation is often made that it works well in checkerboard-type material arrangements. Although this approach works well for a vast majority of LWR reactor problems [2], its shortcomings and limitations can be demonstrated on fixed cross-section benchmarks [14, 16]. The true transverse leakage shape, in particular, may be very complicated. As a result, the simple three-node fit typically breaks down in the following cases:

- Near external boundaries of the reactor, and typically in reflector nodes near the boundary where the flux gradient due to thermalization is sharper than the quadratic approximation could match. In such cases the numerical scheme could lead to negative fluxes, which in turn may destabilize the entire calculation and lead to non-convergence [2]. In these reflector areas, node-averaged errors of up to 10% in flux is not unusual for the quadratic leakage approximation, and may be substantially larger if convergence problems occur.
- At sharp material changes, as would be the case near control rod positions [18]. In turn, such errors could lead to the misprediction of important safety parameters such as control

rod worths. At such interfaces, errors in node averaged power distribution of between 3problems.

- In adjacent nodes which have very different sizes, or within nodes with large aspect ratios. This deficiency places a restriction on the code user with respect to the choice of meshing scheme, and in extreme cases, leads to non-convergence of the solution.

These situations occur regularly in power reactors, and especially in research reactor cores with compact, heterogeneous designs.

2. A CONSISTENT QUADRATIC LEAKAGE APPROXIMATION

In this work we aim to develop an approach which improves upon the accuracy of the standard quadratic transverse leakage approximation, but does not substantially degrade the computational efficiency of standard nodal methods. The foundations for such an improved method will be found within the class of higher order nodal methods. The higher order methods have been demonstrated to significantly improve upon the accuracy of the quadratic transverse leakage approximation, but thus far with a large and unacceptable associated computational cost [18][19]. Typically, standard coarse mesh nodal methods provide performance improvement factors of between 100 and 1000 in 3D as compared to finite difference methods. The current status of higher order nodal methods decreases this advantage by a factor of around 30, and hence makes the coarse mesh methods less attractive given the other complications which they introduce, such as coarse mesh burnup and intra-nodal cross-section shape approximations. In this paper, a method is suggested which would aim to maintain the accuracy benefits of the higher order approaches, but mitigate the performance shortcomings.

It should be stated that the class of higher order nodal diffusion methods (briefly described in the upcoming sections), provide not only significant accuracy improvements, but inherently provides information regarding the detailed intra-nodal flux shape, which is needed for features such as homogeneous flux reconstruction. Nevertheless, they have not found acceptance within industry standard codes, mostly due to their performance problems. This work therefore also aims to make this powerful class of solution methods practical for use in production codes.

2.1 The Standard Quadratic Leakage Approximation

The typical standard nodal (zero order nodal) approach entails, as stated, the use of a three-node quadratic fit of the average transverse leakages in order to approximate the shape of the transverse leakage term in the node of interest. In order to clarify this consider the standard nodal diffusion method which requires the solution of a set of nodal balance equations, obtained by integrating the diffusion equation

$$- \bigtriangledown \cdot [D^g(x,y,z) \bigtriangledown \Phi^g(x,y,z)] + \sigma^{g,rem}(x,y,z)\Phi^g(x,y,z) - Q^g(x,y,z) = 0 \qquad (1)$$

over the volume of a given node. In eq. (1) $D^g(x,y,z)$ denotes the diffusion coefficient, $\Phi^g(x,y,z)$ the flux in energy group g, $\sigma^{g,rem}(x,y,z)$ the removal cross-section and $Q^g(x,y,z)$ the group source comprising both the scattering and fission sources within the node. The balance equation (2) for a given node n may thus be expressed as

$$\sum_{j=1}^{6} a_n^{nj} \overline{J}_{jn} + \sigma_n^{rem} \overline{\Phi}_n = Q_n \tag{2}$$

where $\overline{J}_{jn}$ denotes the normal component of the net current on surface between node j and node n (with the normal pointing outward from node n) and a_n^{nj} the surface to volume ratio of that surface. In order to solve the set of balance equations, an auxiliary set of transversely integrated one-dimensional equations is needed to determine the node averaged flux to side-averaged current relationship. These transversely integrated one-dimensional equations contain transverse leakage terms, and are (illustratively for direction x and group g) given as

$$-D^g \frac{d^2}{dx^2}\phi^g(x) + \sigma_{rem}^g \phi^g(x) = \chi^g \frac{1}{k_{eff}} \sum_{h=1}^{G} \phi^h(x)\nu^h \sigma_{fis}^h + \sum_{h=1, h\neq g}^{G} \phi^h(x)\sigma_{scat}(h \to g) - L^{g,yz}(x) \ . \tag{3}$$

Here the source term has been fully expanded and χ^g denotes the fission spectrum, ν^g the number of neutrons released per fission, σ_{fis}^h the fission cross-section, $\sigma_{scat}(h \to g)$ the scattering cross-section and $L^{g,yz}(x)$ the transverse leakage term which appears due to the integration of the y - and z- components of the Laplacian term. We have

$$L^{g,yz}(x) = L^{g,y}(x) + L^{g,z}(x)$$

$$= \frac{1}{h_y}\left(J^{g,y}(x, \frac{h_y}{2}) + J^{g,y}(x, -\frac{h_y}{2})\right) + \frac{1}{h_z}\left(J^{g,z}(x, \frac{h_z}{2}) + J^{g,z}(x, -\frac{h_z}{2})\right) \tag{4}$$

or more formally in terms of the flux

$$L^{g,yz}(x) = -D^g \left[\frac{1}{h_y}\frac{1}{h_z}\int_{h_y h_z}\left(\frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2}\right)\phi^g(x,y,z)dydz\right] \ . \tag{5}$$

In these equations h_x refers to the node size in the $x-$direction (analogously for y and z).

In the standard quadratic leakage approximation, eq. (5) is approximated by fitting the average value, $\overline{L}^{g,yz}(x)$, given by

$$\frac{1}{h_x}\int_{h_x} L^{g,yz}(x)dx = \frac{1}{h_y}\left(\overline{J}^{g,y}(\frac{h_y}{2}) + \overline{J}^{g,y}(-\frac{h_y}{2})\right) + \frac{1}{h_z}\left(\overline{J}^{g,z}(\frac{h_z}{2}) + \overline{J}^{g,z}(-\frac{h_z}{2})\right) \tag{6}$$

over three adjacent nodes in the $x-$direction to obtain a constant, linear and quadratic term in the central node.

2.2 Existing Higher Order Approaches

In the past, higher order nodal methods have been suggested [18, 19, 22] to address this shortcoming. In principle, higher order nodal equations provide a consistent description of the intra-nodal flux shape and hence remove the need to approximate the transverse leakage term. This

is achieved by expressing the intra-nodal flux as a multi-variate expansion and projecting the solution onto a set of Legendre polynomials in each direction.

As a starting point, we will follow the steps utilized in these higher order approaches, but thereafter make a number of important assumptions and decisions in order to formulate a practical scheme for expressing the transverse leakage term in a consistent manner - in other words use information naturally available from the nodal solution. In higher order nodal methods, in three dimensions, the intra-nodal flux shape is typically expanded as:

$$\phi^g(x,y,z) = \sum_{l=0}^{L}\sum_{m=0}^{M} f_{lm}(x)P_l(\frac{2y}{h_y})P_m(\frac{2z}{h_z}) + \sum_{m=0}^{M}\sum_{k=0}^{K} g_{mk}(y)P_m(\frac{2z}{h_z})P_k(\frac{2x}{h_x}) +$$

$$\sum_{k=0}^{K}\sum_{l=0}^{L} h_{kl}(z)P_k(\frac{2x}{h_x})P_l(\frac{2y}{h_y}) - 2\sum_{k=0}^{K}\sum_{l=0}^{L}\sum_{m=0}^{M} c_{klm}P_k(\frac{2x}{h_x})P_l(\frac{2y}{h_y})P_m(\frac{2z}{h_z}) \tag{7}$$

with $f_{lm}(x), g_{mk}(y)$ and $h_{kl}(z)$ representing one-dimensional semi-moments in each direction and c_{klm} denoting the full flux moments.

All of the semi-moments ($f_{lm}(x)$, $g_{mk}(y)$ and $h_{kl}(z)$) may be related to the full flux moments (c_{klm}) quite simply via

$$c_{klm} = \frac{2k+1}{h_x}\int_{h_x} f_{lm}(x)P_k(\frac{2x}{h_x})dx$$

$$= \frac{2l+1}{h_y}\int_{h_y} g_{mk}(y)P_l(\frac{2y}{h_y})dy$$

$$= \frac{2m+1}{h_z}\int_{h_z} h_{kl}(z)P_m(\frac{2z}{h_z})dz\ .$$

and

$$c_{klm} = \frac{2k+1}{h_x}\frac{2l+1}{h_y}\frac{2m+1}{h_z}\int_{h_x h_y h_z}\phi^g(x,y,z)P_k(\frac{2x}{h_x})P_l(\frac{2y}{h_y})P_m(\frac{2z}{h_z})dxdydz.$$

Here K, L and M represent the order of the method in each direction, and the same value is assumed in each direction (we will use K for all directiions). If we insert this trial function (7) into the expression for transverse leakage (5), we obtain a more rigorous expression for the true transverse leakage shape. As illustration, we present the full expression for the $x-$directional transverse leakage term, and only the contribution from the $y-$direction ($z-$direction has similar form):

$$L^{g,y}(x) = \frac{1}{h_y}\sum_{k=0}^{K}\left(J^{+}_{0k,y} + J^{-}_{0k,y}\right)P_k(\frac{2x}{h_x}) - \frac{2D}{h_y^2}\sum_{k=0}^{K}\left[\left(P_k'(1) - P_k'(-1)\right)\left(f_{k0}(x) - \sum_{l=0}^{K} c_{lk0}P_l\left(\frac{2x}{h_x}\right)\right)\right] \tag{8}$$

where $J^{+}_{0k,y}$ denotes the net current moment of order $(0,k)$ on the top $(+)$ surface in the $y-$direction, or more precisely

$$J^{+}_{0k,y} = -D^{g}\frac{\partial}{\partial y}g_{0k}(y)\mid_{y=+\frac{h_y}{2}} \tag{9}$$

This expression for $L^{g,y}(x)$ decribes the true shape of the transverse leakage in direction x from direction y out of the node in terms of side-current moments, semi-moments in the x-direction and full flux moments. To determine these additional unknowns, a set of higher order balance equations are typically solved.

The full set of higher order equations for these moments may be generated in a number of ways, with typical approaches being either variational [19], or via weighted transverse integration [18]. Independent of the method used, the obtained higher order equations are analogous to equations (2) and (3) in the sense that a balance equation and three one-dimensional auxiliary equations are obtained for each full flux moment, with the solution of the weighted transversely integrated auxiliary one-dimensional equations providing the needed relationships between flux moments and side-current moments. These full flux moments (or expansion coefficients up to the order of the method) are chosen as primary unknowns, with the zero order expansion representing the standard nodal method. It is found that the computational cost of solving for the full set of higher order flux moments grows linearly with the order [18]. The computational cost of these higher order methods, which are capable of reproducing the intra-nodal flux distribution, have limited their use and hence advantage of their accuracy benefits has not been fully taken. This approach produces $(K+1)^3$ balance equations for the full flux moments, and $3(K+1)^2$ auxilliary one-dimensional equations.

2.3 The Proposed Solution

In this work, we will make an effort to represent the transverse leakage expression without solving the full set of higher order nodal equations. If we analyse the full expression of transverse leakage (8) for various orders of the method, we may notice:

- If, in expression (8), $K = 0$, we obtain the standard zero order flat leakage approximation:

$$L^{g,y}(x) = \frac{1}{h_y}\left(J^{+}_{00,y} + J^{-}_{00,y}\right).$$

The average leakages in three adjacent nodes are typically utilized in the standard zero order nodal methods to approximate the leakage polynomial via a quadratic fit.

- If $K \to \infty$ and using the definition of $f_{k0}(x)$, we obtain:

$$L^{g,y}(x) = \frac{1}{h_y}\sum_{k=0}^{K}\left(J^{+}_{0k,y} + J^{-}_{0k,y}\right)P_k(\frac{2x}{h_x})$$

.

- For any practical application $0 < K < \infty$, and we may rewrite

$$L^{g,y}(x) = \frac{1}{h_y}\sum_{k=0}^{K}\left(J^{+}_{0k,y} + J^{-}_{0k,y}\right)P_k(\frac{2x}{h_x}) - \frac{2D}{h_y^2}\sum_{k=0}^{K}\left[\left(P_k^{'}(1) - P_k^{'}(-1)\right)\right]\sum_{l=K+1}^{\infty} c_{lk0}P_l\left(\frac{2x}{h_x}\right) \tag{10}$$

.

It can be seen that if we limit the leakage to a second order polynomial expansion with $K = 2$ (and use the fact that $\left(P_k^{'}(1) - P_k^{'}(-1)\right) = 0$ for both $k = 0$ and 1), the second term in eq. (10) does not contribute (index l starts at 3). Hence, if we limit $L^{g,y}(x)$ to a second order expansion we obtain expression (11) and we have formulated what may be termed the consistent quadratic leakage approximation, written here with contributions from both y and z as

$$L^{g,yz}(x) = \frac{1}{h_y}\sum_{k=0}^{2}\left(J^{+}_{0k,y} + J^{-}_{0k,y}\right)P_k(\frac{2x}{h_x}) + \frac{1}{h_z}\sum_{k=0}^{2}\left(J^{+}_{k0,z} + J^{-}_{k0,z}\right)P_k(\frac{2x}{h_x}) \tag{11}$$

.

This expansion is still of the second order, and we aim, in this phase of the work, simply to improve the representation of the leakage term as compared to the standard approach, and not necessarily to increase the order of the approximation. We notice that in this consistent, higher order leakage approximation, the transverse leakage terms may be expressed as a function of one-dimensional current moments ($J^{+}_{0k,y}$ and $J^{+}_{k0,z}$). Our task therefore is reduced to finding a method of generating these higher order moments, and touse them in the construction of the zero-order transverse leakage shape.

As is typically done in higher order methods, we resort to the weighted transverse integration procedure to generate a set of one-dimensional equations which may be solved to generate the current moments needed in eq. (11).

Transverse integration requires that eq. (1) is integrated over the two transverse directions, in order to produce a one-dimensional equation in the third direction. This process is repeated for all three directions. To achieve this it is convenient to adopt the notation of three arbitrary direction (u, v, w), with u representing the direction of choice and v and w the transverse directions. To produce the set of transversely integrated, one-dimensonal, higher order nodal equations in terms of (u, v, w), eq. (1) is multiplied by Legendre polynomials in both transverse directions, of order k and l, respectively. We let k and l range from 0 to K for all combinations of (k, l), where K denotes the order of the method. Note that $K = 0$ denotes the standard lower order equations. Furtermore, I will denote the maximum source expansion order used to represent the sources in the individual one-dimensional equations and will be set to 4 in this implementation. Hence, a specific higher order solution is classified by both indices (K, I). The resulting equation, after begin transversely integrated over w and then v, looks similar to the standard zero order one-dimensional equations, but now with one-dimensional flux moments as primary unknowns. The obtained one-dimensional higher order equation is given in (12) as

$$-D\frac{d}{du^2}\phi^{wv,g}_{kl}(u) + \sigma_{rem}\phi^{wv,g}_{kl}(u) = \chi^g\frac{1}{k_{eff}}\sum_{h=1}^{G}\phi^{wv,h}_{kl}(u)\nu^h\sigma^h_{fis} + \sum_{h=1}^{G}\phi^{wv,h}_{kl}(u)\sigma^h_{scat}(h \to g) - L^{wv}_{kl}(u) \tag{12}$$

with

$$L_{kl}^{wv}(u) = L_{kl}^{wv,v}(u) + L_{kl}^{wv,w}(u) \tag{13}$$

as the higher order transverse leakage contributions from v and w, respectively.

In this notation the subscripts and superscripts respectively denotes the orders and directions over which a quantity has been integrated. Since, according to eq. (11), in direction u, we are only interested in (k,l) pairs of $(0,0),(0,1),(0,2),(1,0)$ and $(2,0)$, and thus only these equations need to be generated.

This implies that limiting the leakage expansion to order 2 and only solving the higher order equations needed for representation of the transverse leakage term reduces the number of additional, one-dimensional higher order equations from 27 to 15 in 3D (if we include the zero order 1D equations). This is the second important simplification as compared to full higher order approaches.

After we perform the weighted transverse integration and obtain one-dimensional equations (eq. 12), we will proceed to solve these equations analytically, as is typically done in the ANM zero order method. From the analytic solution, we will obtain the needed current moments by solving two-node problems in each direction (as is also typically done in zero order methods). The major difference in these higher order equations (as compared to the zero order equations), is the structure of the higher order transverse leakage terms (13). These terms are still quite complicated and contain various current, sideflux and full flux moments. Here, however, we make an important observation. The average value of the leakage terms in the higher order equations, as given in (14) for direction u and contribution from w, is

$$\begin{aligned}\overline{L}_{kl}^{wv,w} &= \frac{2k+1}{h_w}\left(J_{l0}^{w}(\frac{h_w}{2}) + (-1)^k J_{l0}^{w}(-\frac{h_w}{2})\right) \\ &+\frac{D(2k+1)k(k+1)}{h_w^2}\left(\phi_{l0}^{vu,w}(\frac{h_w}{2}) + (-1)^k \phi_{l0}^{vu,w}(-\frac{h_w}{2})\right) - \frac{2D(2k+1)k(k+2)}{h_w^2}\phi_{0l0}^{wv}.\end{aligned} \tag{14}$$

where ϕ_{lk} refers to side flux moments and ϕ_{klm} to full flux moments. The above expression may be constructed from quantities which are already available within our solution. In order to explain this, consider:

- when $l = 0$ all quantities are from the standard zero order nodal solution - namely surface-averaged net currents (J_{00}^{w}) , surface-averaged fluxes ($\phi_{00}^{vu,w}$) and node-averaged flux (ϕ_{000}^{wv})
- when $l > 0$, then $k = 0$ and eq. (14) reduces to

$$\overline{L}_{0l}^{wv,w} = \frac{1}{h_w}\left(J_{l0}^{w}(\frac{h_w}{2}) + J_{l0}^{w}(-\frac{h_w}{2})\right). \tag{15}$$

  However, these surface current moments will be available since the equation pairs were already identified as necessary to be solved for expressing the zero order transverse leakage term in expression (11).

This implies that a "flat leakage" approximation in the higher order equations allows us to resolve the higher order leakage terms without the need for solving any further equations. This

is the third important assumption which differentiates this method from the typical higher order approach.

At this point we make a final important observation. In order to solve the higher order one-dimensional equations and thus to obtain the current moments which we require in the zero order transverse leakage expression (eq. 11), we construct a two-node problem utilizing current and flux moment continuity conditions at shared interface surfaces and solve for the interface current moments. This approach is analogous to the standard zero order ANM and requires the average value of the flux moment under consideration. In full higher order methods, the average value of the flux moments are obtained from a full spatial sweep of the system for each moment, and this step is the primary reason for the computational burden incurred by these methods. If we, once again, inspect the set of equation pairs needed to represent only the zero order transverse leakage term, we identify that, for the u direction, we require node-averaged flux moments with indices (000,001,002,010,020). All of these one-dimensional flux moments are typically calculated by nodal codes by projecting the one-dimensional analytic solutions onto a set of Legendre Polynomials, and hence are already available. It is thus not needed to sweep the system to obtain these flux moments, and the subsequent current moments from the solution of the constructed two-node problems. This approach does however imply that these higher order moments do not exhibit long range nodal coupling, and that resolving them from two-node problems in every direction is sufficient.

Nevertheless, this observation of using the one-dimensional flux moments obtained from any typical nodal code instead of sweeping the system for their average values, is the final differentiating factor between the described method and the full higher order methods, and is the primary reason why this formulation could prove to be the basis for a practical consistent higher order transverse leakage approximation.

In summary, the proposed method adapts the typical higher order nodal diffusion method in the following ways:

- limit the order of the transverse leakage expansion in the zero order equations to 2. The resulting expression is exact and requires only one-dimensional current moments on each surface;
- apply a "flat" leakage approximation in the higher order one-dimensional equations. This approximation effectively neglects cross-terms from the solution of the higher order equations;
- instead of sweeping the system, obtain the node-averaged values for the higher order flux moments from the zero order nodal solution. This is possible since only a subset of current moments (as compared to full higher order) are needed to express the zero-order transverse leakage term, and specifically only higher order moments with a single non-zero index;
- solve a two-node problem on each surface to obtain the current moments from the analytic solution of the one-dimensional higher order equations.

3. RESULTS AND DISCUSSION

The described method was implemented within an ANM based nodal test code in order to compare the performance and accuracy against the standard quadratic leakage approximation, as well as against a full higher order (limited to second order) method. Two problems, in both their 2D and 3D representations, are calculated and compared. The first is the two-group MOX mini-core C5 benchmark problem [15] and the second the well-known two-group IAEA LWR benchmark problem [14]. Comparitive results for the various transverse leakage approaches are presented. A fourth order expansion is used for the one-dimensional fission and scattering sources in all cases.

3.1 OECD/NEACRP Two-group MOX C5 Benchmark Problem

We present in this section results for the 2D [15] and 3D [16] versions of the well known MOX C5 benchmark problem. Two-group homogeneous cell cross-sections were specified in [15]. Assembly homogenized cross-sections are obtained from pin cell data using a discrete ordinate calculation (TWODENT [17] on the spatial mesh 132×132 and S_{16} quadrature set) for each assembly with reflecting boundary conditions. Results obtained for the 2D and 3D versions of the problem are presented in Tables I and II, respectively. The reference solution to these problems were obtained with 16 times refined zero order nodal calculations. In these tables SQLA refers to the Standard Quadratic Leakage Approximation, CQLA to the proposed Consistent Quadratic Leakage Approximation and FULL-HO (2) to a full higher order (limited to order 2) solution.

Table I: Results for the 2D, two-group MOX C5 benchmark problem

	Reference	SQLA	CQLA	FULL-HO (2)
Eigenvalue	0.942738	0.942896 (17pcm)	0.94261 (12pcm)	0.942683 (5 pcm)
Max. nodal power error	—	0.59%	0.16%	0.05%

Table II: Results for the 3D, two-group MOX C5 benchmark problem

	Reference	SQLA	CQLA	FULL-HO (2)
Eigenvalue	0.94024	0.94060 (38 pcm)	0.94029 (5 pcm)	0.94032 (7pcm)
Max. assembly power error	—	0.36%	0.27%	0.40%
Max. nodal power error	—	0.58%	0.48%	0.56%

We note from the results for the 2D and 3D versions of this problem that CQLA maintains an excellent accuracy in eigenvalue and power distribution. Quadratic leakage is still reasonably accurate, but exhibits a larger error in eigenvalue for the 3D problem. From this problem we may deduce that the CQLA approach performs similarly to a full higher order (limited to second order) method in 2D and 3D, and that the "flat" leakage approximation in the higher order equations does not prove too penalising. In order to evaluate the computational cost of CQLA as compared to SQLA and full higher order (2nd order), we investigate the larger IAEA LWR problem in both 2D and 3D in the next section.

3.2 IAEA LWR Two-group Benchmark Problem

This benchmark problem is widely known and used to evaluate and compare diffusion solvers. Reference results for the problem, in terms of both eigenvalue and power distribution are obtained from the original benchmark publication [14] which utilized an extrapolated fine-mesh finite difference technique. We firstly present results from the 2D version of the benchmark.

Table III: Results for the 2D, two-group IAEA LWR benchmark problem

	Reference	SQLA	CQLA	FULL-HO (2)
Eigenvalue	1.029585	1.02961 (3pcm)	1.02960 (2pcm)	1.02959 (0 pcm)
Max. nodal power error	—	0.90%	0.17%	0.21%
Computational cost factor	—	1.0	2.1	5.0

In Table III results for the 2D version of the benchmark indicate that, although the Standard Quadratic Leakage Approximaton (SQLA) is already relatively accurate for this problem, the Consistent Quadratic Leakage Approximation (CQLA) improves significantly upon the maximum nodal power error. This improvement is similar to what is found for a full higher order solution (also limited to second order), but at a reduced computation cost. It can be noted that the computational burden for the full higher order solution is also not too penalizing for this relatively small 2D problem. In the SQLA, the transverse leakage representation is obtained from solving for three coefficients in each coordinate direction, whilst in the CQLA (in 3D), 4 two-node problems have to be solved on each surface in a given direction. For a full higher order solution, 27 flux moments are typically solved via inner spatial iterations. It should thus be clear that the CQLA approach, although much less computationally expensive than full higher order solutions, would remain somewhat more expensive than SQLA.

In order to test the approach on more realistic problems, and to obtain a better indication of the computational burden, we move to the 3D version of this benchmark, for which results are presented in Table IV.

Table IV: Results for the 3D, two-group IAEA LWR benchmark problem

	Reference	SQLA	CQLA	FULL-HO(2)
Eigenvalue	1.02903	1.02911 (8pcm)	1.02908 (5pcm)	1.02908 (5pcm)
Max. assembly power error	—	1.48%	0.64%	0.77%
Max. nodal power error	—	2.90%	2.02%	1.88 %
Computational cost factor	—	1.0	1.7	9.4

The 3D version of the problem still shows excellent agreement for all the approaches in eigenvalue. Nevertheless, a marked improvement in the maximum assembly averaged powers is observed for the CQLA method. We notice that the CQLA method has improved in efficiency for the larger problem, especially if we consider that a full higher order 3D solution (limited to order 2) to this problem exhibits a computational cost factor of 9.4. However, a large localized nodal error is reported by all methods. Table V analyses the distribution of these errors by tabulating the layer averaged and layer maximum power errors for all fuel layers in the system for the SQLA and CQLA approaches.

Table V: Axial layer power errors for the IAEA-3D problem

Layer	SQLA Ave(Max)	CQLA Ave(Max)	Layer	SQLA Ave(Max)	CQLA Ave(Max)
2	**1.59 (2.90)**	**1.34 (1.82)**	11	0.51 (1.13)	0.31 (0.62)
3	0.55 (1.74)	0.31 (0.80)	12	0.50 (1.17)	0.29 (0.65)
4	0.47 (1.48)	0.28 (0.54)	13	0.49 (1.22)	0.27 (0.54)
5	0.46 (1.32)	0.29 (0.63)	14	0.46 (1.28)	0.26 (0.49)
6	0.49 (1.22)	0.33 (0.68)	15	0.45 (1.37)	0.24 (0.58)
7	0.50 (1.16)	0.34 (0.68)	16	0.43 (1.50)	0.27 (0.73)
8	0.52 (1.13)	0.34 (0.73)	17	0.52 (1.71)	0.43 (0.99)
9	0.53 (1.13)	0.34 (0.71)	18	**1.60 (2.70)**	**1.60 (2.02)**
10	0.52 (1.10)	0.32 (0.64)			

From Table V we may gain a better understanding of the strengths and shortcomings of the proposed CQLA method. In all layers of the system CQLA improves upon SQLA by approximately a factor of 2, with the exception of the outer fuel layers adjacent to the axial reflectors. These errors can occur either due to the insufficient leakage order (limited in both cases to order 2), or due to the lack of cross terms in the intra-nodal flux expansion. In the CQLA approach this cross-term limitation is as a result of the "flat" leakage assumption in the higher order equations. An analysis of the error profile of the full higher order solution (FULL-HO (2)) exhibits exactly the same error distribution (maximum errors in top and bottom fuel layers) and hence we may deduce that, since all cross-terms are included in the full higher order solution, these larger errors are as a result of an insufficient flux expansion order. The CQLA method will therefore provide significant improvement in accuracy as compared to SQLA, but only in regions where the leakage shape is approximately quadratic in nature. Future work would therefore include the extension of this approach to higher orders, while retaining the concepts of only calculating the quantities needed by the zero-order transverse leakage sources and utilizing information already available from the zero order solution.

From both the investigated problems we may deduce that the CQLA approach retains most of the accuracy advantages of full higher order methods, but at a much reduced computation cost. It is foreseen that the method will be packaged in a standalone transverse leakage module, which may be easily coupled to any existing nodal code. It is expected that the reduced overhead and memory usage of such a standalone module could potentially improve the performance of the CQLA method even further, and establish it as a viable and practical alternative to the standard quadratic transverse leakage approximation.

4. CONCLUSION

Standard, or zero-order, nodal diffusion methods are extensively used in power and research reactor calculational industries. Specifically in the transverse integrated variants of nodal methods the well-known quadratic leakage approximation is the primary source of error. In this work, a method is proposed which entails the use of an accurate, yet practical, higher order-based formulation to represent the one-dimensional transverse leakage terms. This "Consistent" quadratic leakage approximation eradicates most of the shortcomings produced by the standard three-node quadratic leakage approximation and improves power distributions significantly in

regions where the transverse leakage shape is quadratic in nature. In the case of the IAEA-3D LWR benchmark problem, the maximum assembly average power error is improved from 1.48% to 0.64%, with an associated increase in computional cost by a factor of 1.7, as compared to full higher order methods (second order) which require almost 10 times more computational time. The method should be easily implemented within any existing zero-order nodal code, with the only requirement that the moments of the one-dimensional solutions within each node are available. Future work would entail the inclusion of higher order approximations (higher than second order) to the leakage shape, the potential inclusion of cross-terms and the application of the method to generate fine mesh fluxes from the available intra-nodal information.

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