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Investigating Diffusion Coefficient Anisotropy in Axially Heterogeneous High Conversion Water Reactors

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Abstract - *High Conversion Water Reactors such as the Hitachi RBWR generally have highy axially heterogeneous cores with alternating layers of fissile and fertile material. A new method of generating anisotropic diffusion coefficients in the Monte Carlo code Serpent is used to investigate the extent of anisotropy arising from this structure and the effect of their utilisation on the quality of diffusion calculation results. It was found that whilst the method does capture some anisotropy arising from the axial heterogeneity, they do not lead to improved diffusion calculation results for the RBWR assembly under consideration.*

I. INTRODUCTION

High Conversion Water reactors have a conversion ratio of greater than unity, in contrast to typical light water reactors (LWRs). This is achieved by reduced moderation of neutrons, resulting in a faster neutron spectrum than is generally seen in an LWR. This allows them to achieve some of the Generation IV goals, in particular fuel sustainability and the ability to burn the transuranic elements in spent LWR fuel, but whilst making use of more mature LWR technology. The Hitachi RBWR (Resource-renewable Boiling Water Reactor) is one such reactor. The core of this reactor consists of axially alternating layers of fissile and fertile material and therefore has a much higher level of axial heterogeneity than a typical LWR. This heterogeneity produces difficulties in computer modelling and a reliance on axial discontinuity factors for satisfactory neutron diffusion calculations[1].

It is suggested that the use of directional, that is, anisotropic, diffusion coefficients would capture more of the physical reality of the system under consideration. If this results in improved diffusion calculations, it could reduce or remove the contribution to axial discontinuity factors of anisotropy in the diffusion coefficient. The use of discontinuity factors has been commonplace for some time to correct for errors arising in the homogenisation process[2]. However, there are multiple sources of error which could be captured by discontinuity factors. If anisotropy in the diffusion coefficient is one such source of error, it is worthwhile attempting to reduce this error such that discontinuity factors are as close to unity as possible.

This work uses the Monte Carlo code Serpent [3] to generate both isotropic and anisotropic diffusion coefficients for a simplified RBWR assembly, as shown in Figure 1. Diffusion calculations are then carried out using an OpenFOAM-based diffusion solver referred to as *fluxSolver*.

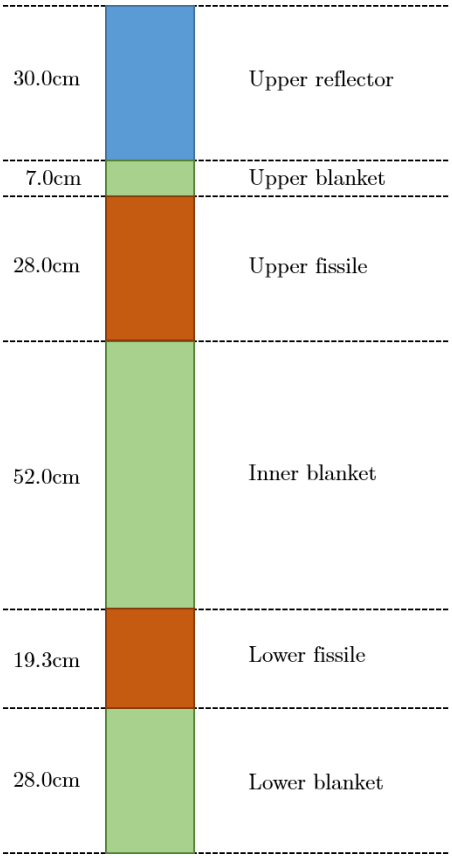


Fig. 1: Simplified RBWR assembly

II. THEORY

In the description of neutron diffusion, it is common to assume that materials, or homogenised regions of a reactor, are isotropic with respect to diffusion and to therefore adopt a single diffusion coefficient, D, for each energy group. It is possible to relax this assumption and provide a fuller description of diffusion via an anisotropic diffusion tensor of the form:

$$\mathcal{D} = \begin{bmatrix} D_{xx} & 0 & 0 \\ 0 & D_{yy} & 0 \\ 0 & 0 & D_{zz} \end{bmatrix}$$

There are two contributions to anisotropy in the diffusion coefficient. The first is the physical anisotropy of the system. For example, the arrangement of fuel pins running along the axis of the reactor results in a different experience for neutrons travelling radially versus axially. The second contribution could be called the 'neighbour effect'. This refers to the impact on the diffusion coefficient due to proximity to a boundary with a diffferent material.

The use of anisotropic diffusion coefficients to treat near-boundary areas is not new. For example, the use of Benoist's method of generating anisotropic diffusion coefficients [4] has been used to model axially heterogeneous fast reactors [5].

Isotropic diffusion coeffiicents are produced as standard in Serpent, whilst the method for producing anisotropic diffusion coefficients is a recent development. This method is derived in [6], then modified in [7]. This method attempts to produce a diffusion coefficient by considering how to sample a flux gradient and a current over an arbitrary surface (the ratio of these two quantities being the diffusion coefficient, in accordance with Fick's Law). The core of this method is the consideration of a neutron travelling from an arbitrary point to an intersection with an arbitrary surface. By considering the flux and current associated with this neutron, it can be shown that a special score can be made at each surface crossing for the diffusion coefficient along the normal to the surface, n:

$$D_n = \frac{R}{2 + R\Sigma_t|_R}$$

where R is the distance travelled from the starting point to the surface and $\Sigma_t|_R$ is the total cross section evaluated at the crossing point. However, this 'diffusion coefficient' is unnormalised since it only considers a single neutron, whereas fluxes and currents are a result of cumulative contributions from many neutrons. Therefore, the average value of D_n needs to be related to some other quantity. Under the strong assumption of an infinite homogeneous medium and isotropic flux it was shown that it is possible to relate $\langle D_n \rangle$ to the total cross section:

$$\langle D_n \rangle = \frac{\alpha}{\Sigma_t}$$

where α is a constant. In [7] it was pointed out that one can alternatively directly tally the total cross section upon surface crossings, resulting in a current-weighted total cross section $\langle \Sigma_t \rangle|_{\mathbb{J}}$. In order to test the performance of the estimator D_n, an intermediate solution was adopted, using an interpolation between the two methods such that the total cross section used is:

$$\langle \Sigma_t \rangle = (1 - m)\frac{\alpha}{\langle D_n \rangle} + m\langle \Sigma_t \rangle|_{\mathbb{J}}$$

The value of the interpolation constant m, also referred to as the *mixing parameter*, was chosen using a 1-D heterogeneous example, generating 24 energy group cross section sets and determining the value of m that allows the best agreement with reference Serpent results for k_{eff} and the axial power distributions. Results presented here are based on a value of $m = 1$.

This methodology was developed further in [8]. Here the derivation of diffusion coefficients was extended from just the axial to the radial direction. This was accomplished by the imposition of a regular three-dimensional Cartesian mesh onto the geometry. The resulting planes were then used to score the tallies required to produce directional diffusion coefficients in the x, y and z directions. This method was investigated in the context of a sodium-cooled fast reactor. It was found that the adoption of these anisotropic diffusion coefficients resulted in greatly improved agreement between homogeneous and heterogeneous calculations in terms of k_{eff}-eigenvalue and radial power distribution. There was also an unexpected improvement in the form of a reduced sensitivity of the diffusion coefficients to the choice of energy group structure.

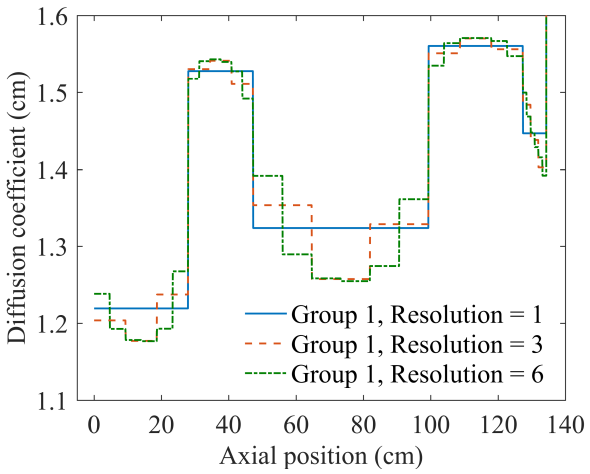


Fig. 2: Fast group diffusion coefficients calculated with different layer resolutions

Further work set out in [9] considered this new method of producing diffusion coefficients in the context of other reactor types. The performance of this method was found to vary strongly between different designs. The design considered that was closest to the RBWR is the VVER, a pressurised water reactor of Russian design with a hexagonal assembly lattice. For this reactor type it was not possible to obtain reasonable agreement with Serpent in terms of k_{eff}.

III. RESULTS AND ANALYSIS

The neighbour effect can be seen in the standard isotropic diffusion coefficients. Figure 2 shows, for a 2-energy group structure, the fast group isotropic diffusion coefficients calculated with each layer of the reactor subdivided into either one, three or six sub-layers (referred to as the layer 'resolution'). All subsequent results are based on a layer resolution of six, since the effect of capturing near-boundary anisotropy is the main area of interest.

The mathematical bases of the two diffusion coefficient formalisms (isotropic vs. anisotropic) are different and therefore one would not necessarily expect them to produce similar values for diffusion coefficients even in the simplest case of infinite, homogeneous materials. Indeed this is found to be the case. The absolute values of the diffusion coefficients produced are certainly different in the case of the RBWR assembly under investigation. This can be seen in Figure 3 which shows the diffusion coefficients calculated under both formalisms.

One would expect that the effect of the neigbouring material would only affect the diffusion coefficient in the direction normal to the interface with that material. This is captured by the anisotropic formalism: as shown in Figure 4, the difference between the axial and radial difffusion coefficients is greatest at the material boundaries.

Calculation method	No. energy groups	k_{eff}	Difference vs Serpent (pcm)
Serpent	n/a	1.09258 ± 0.00002	-
Diffusion (isotropic diffusion coeff.)	2	1.10218	960
	12	1.06978	-2280
	68	1.06986	-2272
Diffusion (anisotropic diffusion coeff.)	2	1.14626	5368
	12	1.06687	-2371
	68	1.06895	-2363

TABLE I: k_{eff} eigenvalue results based on layer resolution of 6 sub layers per layer

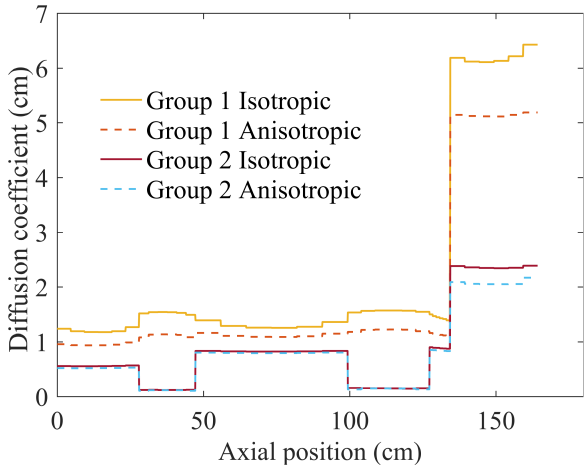


Fig. 3: 2-energy group diffusion coefficients calculated under the isotropic and anisotropic formalisms (for axial direction)

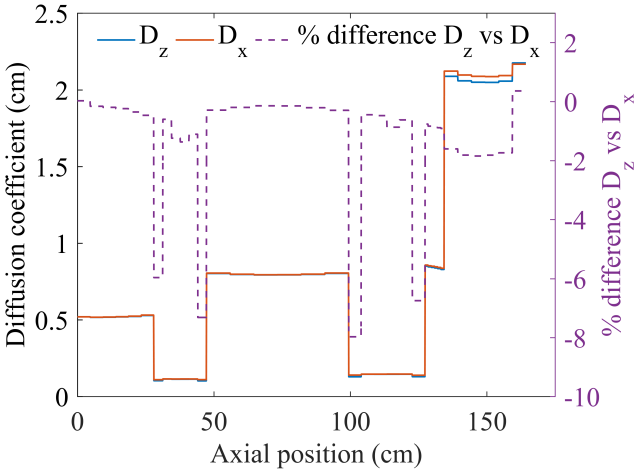


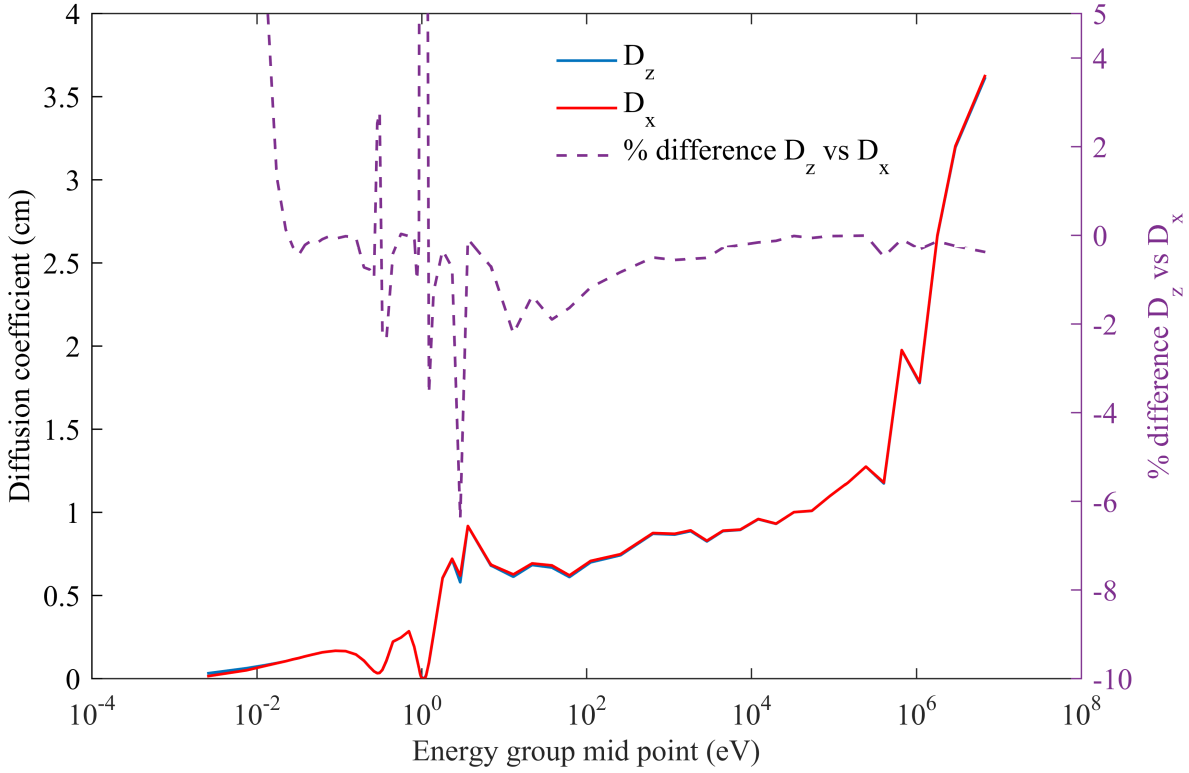
Fig. 4: Thermal group diffusion coefficients in axial and radial directions

The level of anisotropy detected by this formalism appears to depend strongly on energy. Figure 5 shows the radial and axial components of the diffusion tensor plotted against energy, based on a 68 group energy structure for two locations in the assembly. The locations were chosen based on where the greatest level of anisotropy is found, close to material boundaries. Figure 5a shows diffusion coefficients at at height of around 124cm along the assembly, within the upper fissile layer close to the boundary with the upper fertile layer. Figure 5b is based on a height of around 128cm within the upper fertile layer close to the boundary with the upper fissile layer. Some of the sharp increases in anisotropy observed in these graphs could arise from poor statistics where the diffusion coefficient becomes very small. For example, in Figure 5a, the diffusion coefficient approaches zero at around 0.3eV and 1eV. These could be associated with isolated fission resonances in Pu-239 and Pu-240 respectively - noting that the RBWR MOX is assumed to be in its fuel cycle equilibrium composition which contains approximately equal concentrations of these two isotopes. However, in regions of the spectrum with good statistics some dependence on energy can be clearly seen.

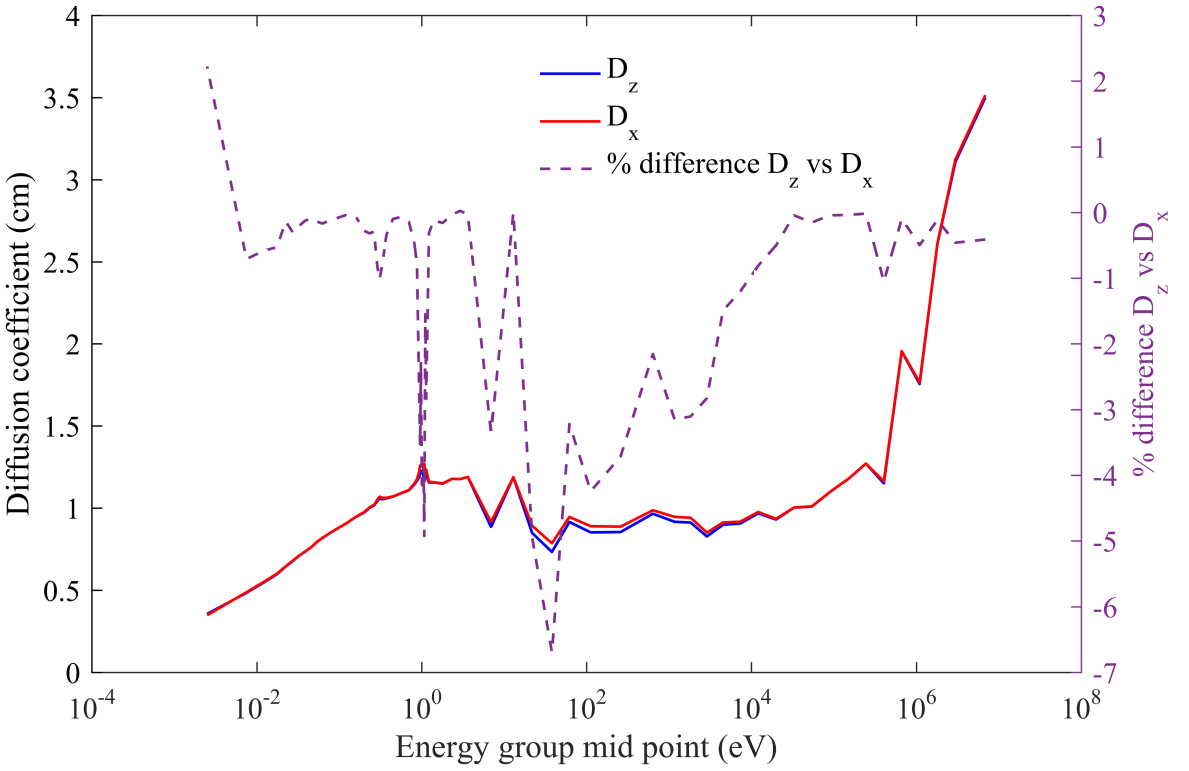
The level of anisotropy is, unsurprisingly, highly variable in the resonance region. Any strong absorption associated with an isotope present in the neighbouring material would be expected to result in a divergence of the axial and radial diffusion coefficients at the energy of the resonance. In the thermal region we see an increasing level of anisotropy with decreasing energy which could be associated with much stronger absorption of thermal neutrons in the fissile region compared with the fertile region. At the higher energies above the resonance region, the level of anisotropy is generally lower. Diffusion is more important at higher energies where diffusion coefficients are largest, which may explain the relatively minor impact of the anisotropic formalism on the results of the 12 and 68-energy group diffusion calculations.

1. k_{eff} Eigenvalue

The performance of the anisotropic diffusion coefficient formalism was analysed using 2, 12 and 68 group diffusion calculations. It was found that the use of the anisotropic diffusion coefficients did not result in better agreement between the diffusion solver and Serpent in terms of the k_{eff} eigenvalue, for any of the three energy group structures, as shown in Table I. The method used to generate anisotropic diffusion coefficients has been tested elsewhere [9] on a number of reactor types. As mentioned previously, it was found that for the light water reactor considered, the corresponding diffusion calculations did not replicate the reference k_{eff} result from Serpent, similar to the situation found here with the RBWR. It is therefore possible that this potential unsuitability for light water reactors may overcome any potential improvements arising from a

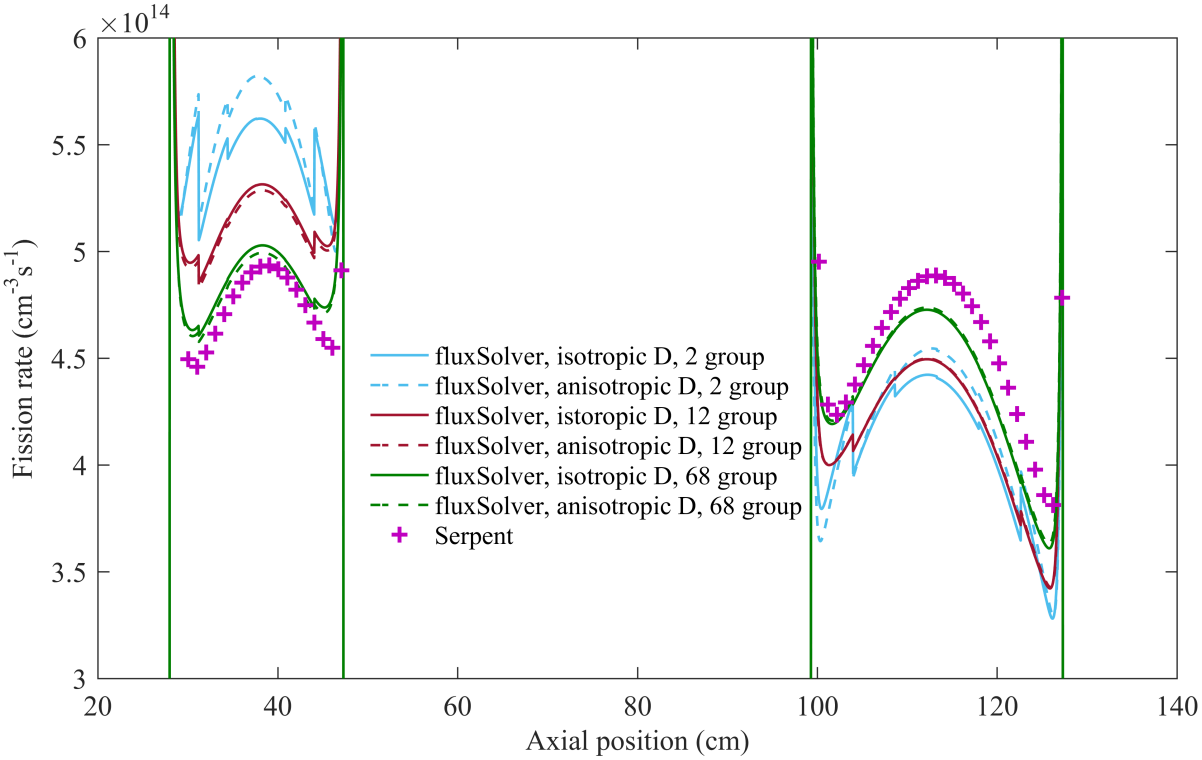


(a) In fissile layer close to boundary with fertile layer

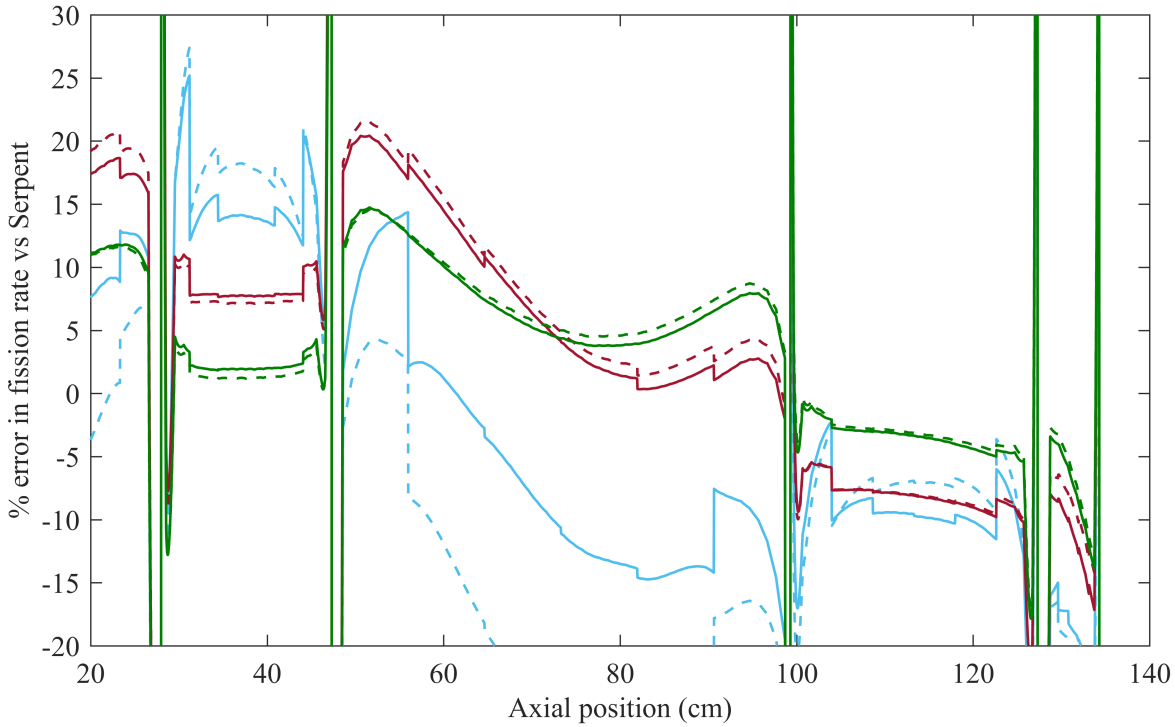


(b) In fertile layer close to boundary with fissile layer

Fig. 5: Anisotropic diffusion coefficient components plotted against neutron energy



(a) Fission rate calculated in both formalisms in 2, 12 and 68 groups and by Serpent



(b) Error in calculated fission rate as compared to Serpent

Fig. 6: Fission rate profile and error as measured against Serpent

fuller treatment of anisotropy in the diffusion coefficient.

2. Flux and Power Profiles

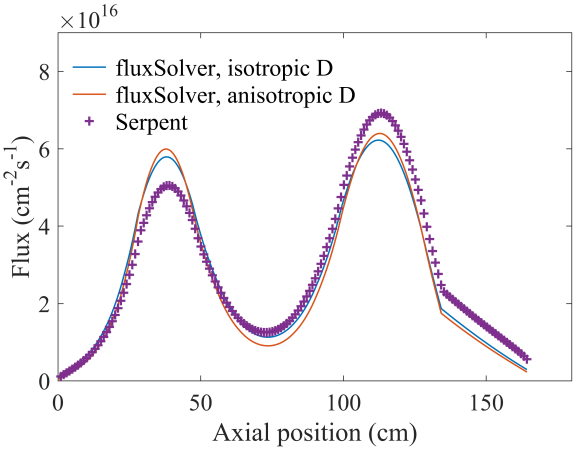


Fig. 7: Fast group flux profile in 2-energy group calculation

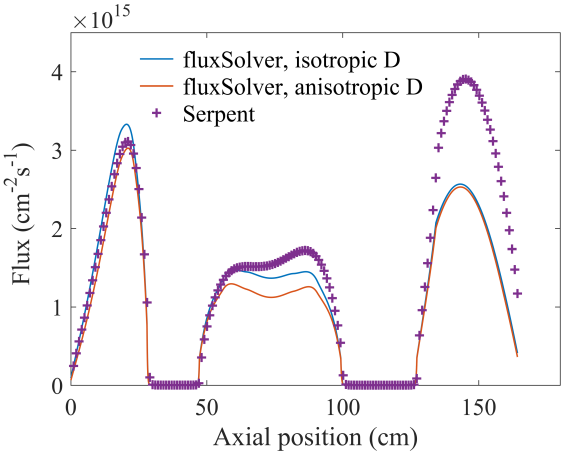


Fig. 8: Thermal group flux profile in 2-energy group calculation

Figure 6 shows the fission rate in the two fissile layers under all three energy group structures, whilst Figures 7 and 8 show the fast and thermal group fluxes respectively, as calculated by the diffusion solver under both diffusion coefficient formalisms and Serpent. As can be seen, the 2-energy group diffusion calculations under either of the diffusion coefficient formalisms do not adequately replicate the flux profiles produced by Serpent. The fission rate profile in the fissile regions of the assembly gives more detail on the differences in results between the two formalisms.

Of particular interest is the fact that the fast flux and fission rate have been overestimated in one of the assembly's fissile layers and underestimated in the other. In this context, the apparently good agreement in terms of k_{eff} of the isotropic formalism in two energy groups would appear to result from a cancellation of errors. Specifically, power is overestimated in one region of the reactor and underestimated in another region. In this light, neither formalism appears satisfactory in two energy groups.

Increasing the number of energy groups progressively improves the agreement with Serpent in terms of the fission rate profile which can be seen clearly in Figure 6. Moving from the isotropic to the anisotropic formalism has the greatest effect on the 2-energy group diffusion calculation, although the error in terms of fission rate is increased in the lower fissile zone and increased in the upper fissile zone.

IV. CONCLUSIONS

The anisotropic diffusion coefficient formalism utilised here appears capable of capturing some of the anisotropy in the diffusion coefficient that arises from the presence of nearby materials. However, based on the results obtained for the simplified RBWR assembly considered, this formalism does not provide better results in terms of k_{eff} eigenvalue or flux/fission rate profiles than the standard isotropic formalism of Serpent. However, this should not preclude further investigation of the potential utility of an anisotropic diffusion coefficient formalism for modelling reactors of this sort. It has been noted elsewhere [9] that this particular method of generating diffusion coefficients may not be compatible with light water reactors, but it is possible that it could be modified to reduce or remove this limitation.

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