2021 International Nuclear Atlantic Conference – INAC 2021
Virtual meeting, Brazil, November 29 – December 2, 2021

ISBN: 978-65-594-1256-3

Application of Neutron Transport and Diffusion Theories to Homogeneous Media

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1. Introduction

In the past years, the Institute for Advanced Studies (IEAv) has been developing the concept of a nuclear microreactor, known as the Advanced Fast Reactors Technology project (TERRA), that could work as a source of electrical and thermal energy and would be useful in very remote areas, such as in deep sea and outer space.

To promote adequate training for the human resources developing this project, it is helpful to adopt simplified models, with good approximation, which can quickly generate neutron kinetic data for nuclear reactors. This would allow a better comprehension of the neutron dynamics behavior, as well as the influence of the different components and variables that are present in the core. In addition, a large amount of data could be generated, improving the training of post-graduate students who contribute to current IEAv projects, especially TERRA.

In this sense, the chosen simplified methods were the Neutron Transport equations, applied to homogeneous and infinite media, and the Neutron Diffusion theory, also for homogeneous media, with one energy group and cylindrical geometry. Both models were then adapted to C/C++ and compared with some other benchmark solutions, as a way of verifying and validating the codes.

2. Methodology

The Transport Equation model applied to an infinite and homogenized medium can be derived from [1] and is given by Eq. 1 [3].

$$T\psi_\infty = \frac{1}{k_\infty} F\psi_\infty + S\psi_\infty \tag{1}$$

where k_∞ stands for the infinity multiplication factor, ψ_∞ the respective autovector, T the diagonal matrix with the total macroscopic cross sections, S the matrix with the isotropic scattering energy transfer components and F the matrix in which its elements represent the product of the average number of neutrons emitted in the energy group, the respective macroscopic fission cross sections and the fission spectrum. Eq. 1 was then rewritten in the form of Eq. 2 for solving purposes:

$$(T-S)^{-1} F\psi_\infty = k_\infty \psi_\infty \tag{2}$$

In this method, the infinity multiplication factor calculated represents the autovalue solution for the system proposed, whereas the correspondent autovector represents the neutron spectra.

The Multigroup Diffusion theory is represented by Eq. 3.

$$\frac{1}{v_g}\frac{\partial \varphi_g}{\partial t} - \nabla \cdot D_g \nabla \varphi + \Sigma_{tg}\varphi_g(r,t) = \sum_{g'=1}^{G} \Sigma_{sg'g}\varphi_{g'} + X_g \sum_{g'=1}^{G} v_g \Sigma_{fg'}\varphi_{g'} + S_g \tag{3}$$

where v_g represents the average number of neutrons emitted by fission, φ the neutron flux in $cm^{-2}s^{-1}$, t the time in s, D the neutron diffusion coefficient in cm, Σ_t the total macroscopic cross section in cm^{-1}, $\Sigma_{sg'g}$ the macroscopic scattering cross section in cm^{-1} with energy change from group g' to group g, X the fission spectrum, Σ_f the macroscopic fission cross section in cm^{-1}, S_g external sources of neutrons and the

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g index refers to each energy group.

In this work, a single energy group will be utilized as a way to perform quick criticality calculations for homogeneous media, or even the case of a homogenized media in which a core with multiple elements presents single average cross-section values.

All the calculations were performed through C/C++. The codes were verified by using some benchmark problems, as seen in [2]. The inputs needed are the volume fraction of each core component in addition to the number of energy groups considered, the total Σ_t, fission Σ_f and scattering Σ_s from group *j* to group *i* macroscopic cross-sections, the average number of neutrons generated per fission and the spectrum for every energy group and material present in the core. The outputs for the criticality code verification are the infinity multiplication factor k_∞ and the neutron flux ratio for every energy group present in the core.

The multiplicity factor for the transport theory was calculated using the autovalue and autovector method, in which a determinant must be calculated by the cofactor method, so that the problem can be easily adapted to any number of groups desired. The value of k_∞ was searched in order to solve the determinant within a desired accuracy.

In the Diffusion method the multiplicity factor was calculated by Eq. 4:

$$k_\infty = \frac{\nu \Sigma_f}{\Sigma_t - \Sigma_s} \tag{3}$$

The critical radius for a cylinder was calculated through Eqs. 4-6, in which B_m refers to the material Buckling number, *D* to the diffusion coefficient, B_g to the geometric Buckling number, *v0* to the smallest zero of the Bessel function, $\widetilde{R}$ to the extrapolated radius and $\widetilde{H}$ to the extrapolated height (which equals ∞ on an infinite cylinder).

$$B_m^2 = \frac{\nu \Sigma_f - \Sigma_a}{D} \tag{4}$$

$$D = \frac{1}{3 \Sigma_{tr}} \tag{5}$$

$$B_g = \left(\frac{\nu_0}{\widetilde{R}}\right)^2 + \left(\frac{\pi}{\widetilde{H}}\right)^2 \tag{6}$$

3. Results and Discussion

Tables I and II summarizes the results achieved for three particular research reactor problems, as seen in [2]. The first for three one-energy group problems, comparing the results obtained by both approximated methods previously described. The second table illustrates the accuracy of results obtained for the transport theory method applied to a six-energy group research reactor.

As it can be noticed in Table I, the multiplicity factor was very accurately calculated with both methods for all one-energy group homogeneous and infinite media problems. When considering the case of a cylinder, the critical radii found were not so precise, but as these methods are very crude approximations with almost instantaneous results, one could consider the results quite satisfactory. Another reason for the higher differences observed in the critical radius results is that the benchmark values were not calculated in [2], but taken from other benchmark references, and some data used, such as the precise atomic weight of the atoms involved to obtain them is unknown, so this work had to assume some values. The approximation was also somewhat worse for problem 23, which consists of a U-D_2O Reactor, significantly more complex, with unknown values of the atomic weights considered by Ref. [2] and in which the diffusion approximation lead to worse results.

The results shown in Table II are quite good, with very low differences in comparison to the analytical benchmark exact solutions. In fact, one can consider the results completely satisfactory, as it is already an approximate solution, whose objective is to provide quick data for many different core arrangements in little time. The little differences are because the auto vector of the determinant mentioned earlier

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represents the flux ratios, and as the autovalor (k_∞) was not exact, the error was propagated. It is important to note that many other problems with different number of energy groups were also tested with great results.

Table I: Results obtained for a one-energy group research reactor.

Problem	Outputs	Results		
		Benchmark [2]	Transport theory	Diffusion theory
7	k_∞	2.290323	2.290331 (+3.492957.10^{-4}%)	2.290323 (0 %)
	r_c (cm)	4.279960	-	5.281604 (+23.40312 %)
13	k_∞	2.250000	2.250008 (+3.555555.10^{-4}%)	2.250000 (0 %)
	r_c (cm)	5.284935	-	6.022654 (+13.95890 %)
23	k_∞	1.133333	1.133342 (+7.941179.10^{-4}%)	1.133333 (0 %)
	r_c (cm)	16.554249	-	7.346256 (-55.62314 %)

Table II: Results obtained for a six-energy group research reactor.

Outputs	Results		Difference
	Benchmark [x]	Transport theory	
k_∞	1.600000	1.599999	-3.81470.10^{-5} %
Group 5 to 6 flux ratio	0.480	0.480000	0 %
Group 2 to 1 flux ratio	0.480	0.479997	-6.59625.10^{-4} %
Group 4 to 5 & group 3 to 2 flux ratio	0.3125	0.312500	1.83105.10^{-5} %
Group 4 to 6 flux ratio	0.150	0.150000	1.27157.10^{-5} %
Group 3 to 1 flux ratio	0.150	0.149999	-6.42000.10^{-8} %

It is convenient to remember that k_∞ was not exact in the transport theory due to the method chosen, which involves the search for a solution of a determinant as previously mentioned. This could be more precise with a higher time sacrifice, considered unnecessary.

A last reactor, which is worth to be studied as to validate the two methods, is a classic PWR reactor, exactly as the one described in [4]. The sum of the macroscopic cross-sections were taken from the data presented in that work and used to calculate the critical radius and multiplicity factor as a final verification to the codes. The results are expressed in Table IV.

Table IV: Results obtained for a PWR reactor [4].

Outputs	Results		
	Benchmark [4]	Transport theory	Diffusion theory
k_∞	1.0008	0.994081 (-0.67136 %)	0.994073 (-0.67216 %)

ISBN: 978-65-594-1256-3

r_c (cm)	160	-	165.075992 (+3.172495 %)

The results are once again very close. The little difference obtained for the multiplicity factor can be explained by the fact that in [4] the denominator of the formula which calculates k_∞ utilizes Σ_a instead of (Σ_t - Σ_s) and could have numerical differences. As for the critical radius, the different number of decimal places used in [4] and this work could easily propagate and increase the errors observed throughout the equations to obtain the critical radius.

4. Conclusions

This work began with the presentation of the Transport Equation model approximated to homogeneous and infinite media, as well as the Diffusion model, for homogeneous media and one-energy group, that were proposed for criticality calculations.

After being adapted to C/C++, the results were compared to well known benchmark solutions [2] in order to verify and validate the models. The infinity multiplicity factors obtained were almost exact, with very little differences in the transport model due to the chosen method used, which involved the calculation of a determinant, with the advantage of being easily adaptable to any number of energy groups. Naturally, the difference observed on the multiplicity factor in comparison to the benchmark solutions could be reduced with the sacrifice of some computing time. The flux ratios for a larger number of groups were also quite good, with little differences due to the value of k_∞.

The critical radius had larger differences, which could be refined in future studies. But they are certainly successful when it comes to providing a very good idea of the dimensions expected for a core, and in very little time.

Finally, the models proposed proved to be very good in providing notions of the values of some of the parameters present in any core, which could be useful in the formation of new personnel who will work in this area and even for post-graduation programs. The software created could help in the production of a data bank and to allow a better understanding of what changes could be expected in a core when certain parameters are altered.

Acknowledgements

This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001, and also by the TERRA Project – Finance Code 001. Acknowledgments are provided to the Institute for Advanced Studies – IEAv for the use of its Laboratories and Computation Facilities.

References

[1] J. J. Duderstadt, and L. J. Hamilton, *Nuclear Reactor Analysis*, John Wiley & Sons, Inc., New York, United States of America (1976).

[2] A. Sood, R. A. Forster, and D. K. Parsons, "Analytical Benchmark Test Set For Criticality Code Verification", *Progress in Nuclear Energy*, vol. 42, pp. 55–106 (2003).

[3] A. D. Caldeira, "Um Método Aproximado de Cálculo do Espectro de Nêutrons em Células de Reatores", *Anais do XII Encontro Nacional de Física de Reatores e Termo-Hidráulica - ENFIR*, Rio de Janeiro, Brazil (2000).

[4] N.M.A.Athanazio, F.A.Braz Filho, and A. D. Caldeira, "A simplified neutronics model for a Pressurized Water Reactor core based on diffusion theory and one energy group", *Proceedings of the INAC 2019: International Nuclear Atlantic Conference. Nuclear new horizons: fueling our future*, Santos, Brazil (2019).