BJRS
BRAZILIAN JOURNAL OF RADIATION SCIENCES

doi.org/10.15392/2319-0612.2024.2361
2024, 12(2) | 01-21 | e2361
Submitted: 2023-10-06
Accepted: 2024-03-25

A numerical validation between the neutron transport and diffusion theories for a spatial kinetics problem

Zanette [a*], R.; Barichello [b], L. B.; Petersen [c], C. Z.

[a] Instituto Federal de Educação, Ciência e Tecnologia Sul-rio-grandense, 96745-000, Charqueadas, RS, Brazil.
[b] Universidade Federal do Rio Grande do Sul, Instituto de Matemática e Estatística, 91509-900, Porto Alegre, RS, Brazil.
[c] Universidade Federal de Pelotas, Instituto de Física e Matemática, 96001-970, Capão do Leão, RS, Brazil.

*Correspondence: rodrigozanette@ifsul.edu.br

Abstract: In this paper, a comparative analysis of numerical results of the neutron transport and diffusion theories for steady-state and transient multigroup problems is presented. The neutron transport equation is known as the one that best describes the behavior of the neutron population in a nuclear reactor. However, due to the difficulty of working with its complete form, other models are considered as approximations to this equation. One such approximation is the neutron diffusion equation, which uses the Fick's Law. It is well known, however, that the diffusion model may not work well under specific conditions. The objective of this work is to establish a quantitative comparison of numerical results obtained for the K dominant eigenvalue and for the scalar fluxes from the two theories and to analyze the influence of the model on the results.

Keywords: neutron transport theory, neutron diffusion theory, comparative analysis, K dominant eigenvalue.

SBPR

BJRS
BRAZILIAN JOURNAL OF RADIATION SCIENCES

doi.org/10.15392/2319-0612.2024.2361
2024, 12(2) | 01-21 | e2361
Submitted: 2023-10-06
Accepted: 2024-03-25

Uma validação numérica entre as teorias de transporte e difusão de nêutrons para um problema da cinética espacial

Resumo: Neste artigo é apresentada uma análise comparativa dos resultados numéricos das teorias de transporte e difusão de nêutrons para problemas multigrupo em estado estacionário e transiente. A equação de transporte de nêutrons é conhecida como a que melhor descreve o comportamento da população de nêutrons em um reator nuclear. Entretanto, devido à dificuldade de trabalhar com sua forma completa, outros modelos são considerados como aproximações desta equação. Uma dessas aproximações é a equação de difusão de nêutrons, que usa a Lei de Fick. É bem sabido, contudo, que o modelo de difusão pode não funcionar bem em condições específicas. O objetivo deste trabalho é estabelecer uma comparação quantitativa dos resultados numéricos obtidos para o autovalor dominante K e para os fluxos escalares nas duas teorias e analisar a influência do modelo nos resultados.

Palavras-chave: teoria de transporte de nêutrons, teoria de difusão de nêutrons, análise comparativa, autovalor dominante K.

SBPR

1. INTRODUCTION

One of the fundamental requirements for the design of nuclear reactors is to understand the behavior of the neutron distribution, which determines the safe operation of such systems. Consequently, one of the central challenges in reactor research is to predict this distribution in detail.

This problem is primarily addressed by two theories: neutron transport theory and neutron diffusion theory [1, 2, 3]. Both theories study the migration of neutrons in both multiplying and non-multiplying media and obtain the flux distribution in space, time, and energy. It requires knowledge of the characteristics, properties, and microscopic and macroscopic quantities of the physical system, such as cross-sections, material composition, geometry, etc.

The most comprehensive equation that models neutron transport is the linear Boltzmann equation, deduced from the principle of conservation (or balance) of the number of neutrons in a convex volume element. The transport equation, developed by Boltzmann, can be used to describe the distribution in space, energy, propagation direction (angle), and time of neutrons within the core of a nuclear reactor. This distribution governs the behavior of a nuclear reactor; however, the integro-differential equation involves three position variables, two angular variables, one energy variable, and one time variable. It is worth mentioning that it is challenging to solve analytically due to the complexity of the functions and the number of independent variables that define the problem [4]. Therefore, finding analytical solutions to the transport equation is only feasible if the system is simplified or idealized in such a way that a closed-form mathematical solution can be obtained. In the steady-state regime, the flux is considered independent of time. Dealing with spatial

dependence in arbitrary geometry is difficult. What is usually done is to consider an idealized model in slab geometry, and thus, the parameters will depend only on one spatial coordinate.

Additionally, it is easier to derive the transport equation than to solve it. However, under certain conditions, they are treated in the most appropriate way to obtain an exact solution. This simplified version of the transport theory is called diffusion theory. Although the conditions required for the validity of diffusion theory are rarely met in practical reactor problems, its use usually results in a good approximation to the exact solution of the transport equation, and due to its simplicity, diffusion theory is commonly used in global reactor problems [5].

To construct the mathematical model of neutron diffusion, i.e., the neutron diffusion equation, we assume that the angular flux has a weak dependence on angle, meaning it exhibits a linear dependence. This approximation is not satisfactory near boundaries or regions where material properties change drastically within distances comparable to the mean free path of neutrons. It is also unreasonable in the vicinity of localized sources and in strongly absorbing media.

Typically, when studying neutron transport in regions of the domain that are several mean free paths away from sources or boundaries in weakly absorbing media, neutron flux varies little with space. Therefore, the neutron diffusion theory serves as a suitable approximation for the physical phenomenon of transport.

Although there is much literature regarding the differences between theories, to our knowledge, this type of numerical comparison between them is very scarce and seldom addressed through cases in the literature.

It is known that, to make a viable approximation between the neutron current and the scalar neutron flux, simplifications are made to find the classical constitutive relation (Fick's law), in which the neutron current term needs to satisfy some simplifications according to [2]: energy separability throughout the equation; isotropy in the source term; weak angular

flux dependence with direction and temporal variation of current density much slower than collision rate. These simplifications allow approximating the neutron current term with the classical Fick's law.

In this sense, a pathway to a better approximation of neutron diffusion theory would be to propose alterations to Fick's law. The starting point would be to analyze the differences in theories for scenarios of reactor power variation over time and, therefore, to analyze the dynamics of a nuclear reactor, comparing the neutron kinetics equation with the transport equation. One of the questions that arises is what possible modifications or extensions of the kinetics equation could describe a more realistic form of overall temporal evolution of scalar flux.

A starting point to answer this is what could be the precise correlations for minimal error compared to transport results. In this sense, comparisons between theories are necessary at certain crucial points of the reactor, such as near boundaries and material interface regions, where large variations in scalar flux are known to occur over a short time interval.

In this work we will propose a quantitative comparison of the two models: transport and diffusion. The analysis is carried out on solutions to a reactor physics problem in slab geometry, a one-dimensional and heterogeneous medium composed of 7 regions, considering the kinetic model of the neutron diffusion and transport equation. The kinetic equations of the neutron diffusion theory were solved using a nodal formulation along with the Backward Euler method and the kinetic equations of the neutron transport theory were solved using time-dependent discrete ordinates code (TDA) [6].

2. FORMULATION AND METHODS

The spatial kinetic equations in neutron diffusion theory for the one-dimensional case in slab geometry, in a domain Ω contained in ℝ, are written as

$$\frac{1}{v_g}\frac{\partial \phi_g(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left(-D_g(x,t)\frac{\partial \phi_g(x,t)}{\partial x}\right) - \Sigma_{Rg}(x,t)\phi_g(x,t)$$

$$+(1-\beta)\chi_g^p \sum_{g'=1}^{G} \nu_{g'}\Sigma_{fg'}(x,t)\phi_{g'}(x,t)$$

$$+ \sum_{g'=1;g\neq g'}^{G} \Sigma_{sg'g}(x,t)\phi_{g'}(x,t) + \chi_g^d \sum_{p=1}^{P} \lambda_p C_p(x,t), \qquad (1)$$

$$\frac{\partial C_p(x,t)}{\partial t} = -\lambda_p C_p(x,t) + \beta_p \sum_{g=1}^{G} \nu_g \Sigma_{fg}(x,t)\phi_g(x,t),$$

where $x \in \Omega$, $t \in [t_0, \infty]$, t_0 is the initial time, $g = 1{:}\,G$ are the neutron energy groups and $p = 1{:}\,P$ are the delayed neutron precursors families. For each energy group g: $\phi_g(x,t)$ is the neutron scalar flux in $[cm^{-2}\,s^{-1}]$, v_g is the neutron speed in $[cm\ s^{-1}]$, D_g is the diffusion coefficient in $[cm]$, Σ_{Rg} is the removal cross-section in $[cm^{-1}]$, β is the total fraction of delayed neutrons, χ_g^p is the prompt fission spectrum, ν_g is the average number of neutrons emitted by fission, Σ_{fg} is the fission cross-section in $[cm^{-1}]$, $\Sigma_{sg'g}$ is the scattering cross-section from energy group g' to g in $[cm^{-1}]$, χ_g^d is the delayed fission spectrum. For each precursors family p: $C_p(x,t)$ is the delayed neutron precursor concentration in $[cm^{-3}]$, β_p is the delayed neutron fraction and λ_p is the delayed neutron

decay constant in $[s^{-1}]$. In addition to these parameters, β is the delayed neutron fraction, that is defined by

$$\beta = \sum_{p=1}^{P} \beta_p \ . \tag{2}$$

The most common boundary conditions for Eqs. (1) are of the type: Dirichlet, Neumann or Robin, which are written in a general form as

$$a_g \phi_g(x,t) + b_g \frac{\partial \phi_g(x,t)}{\partial x} = 0 \tag{3}$$

where $x \in \partial\Omega$ and $|a_g|+|b_g| < 0$ for a_g and b_g real constants. The initial conditions for the spatial kinetics problem are

$$\phi_g(x,0) = \phi_{g0}(x) \; and \; C_p(x,0) = \frac{\beta_p}{\lambda_p} \sum_{g=1}^{G} \nu_g \Sigma_{fg}(x,0) \phi_{g0}(x) \tag{4}$$

where $x \in \Omega$ and $\phi_{g0}(x)$ are known neutron fluxes (steady state solution).

2.1. Spatial variable

The treatment of the spatial variable that we propose in this section will be applied to both the stationary problem and the kinetic problem. This treatment consists of a nodal integration technique along with approximations of the current densities at the interfaces, as present in REF. [5].

The nodal integration technique consists in dividing the domain into N nodes with constant properties (homogeneous medium). Then in each node (i) of dimension $\Delta x^{(i)}$, $x \in [x_{i-1}, x_i]$, we integrate Eqs. (1) for all $x \in [x_{i-1}, x_i]$ and we divide by $\Delta x^{(i)}$. So, we obtain the average spatial variable in each node: average neutron flux, $\underline{\phi}_g^{(i)}(t)$, and average precursor concentration, $\underline{C}_p^{(i)}(t)$, as

$$\underline{\phi}_g^{(i)}(t) = \frac{1}{\Delta x^{(i)}} \int_{x_{i-1}}^{x_i} \phi_g^{(i)}(x,t)dx \tag{5}$$

and

$$\underline{C}_p^{(i)}(t) = \frac{1}{\Delta x^{(i)}} \int_{x_{i-1}}^{x_i} C_p^{(i)}(x,t)dx. \tag{6}$$

In addition, we are still left with the neutron current densities at the node interfaces

$$J_g^{(i)}(x,t) = -D_g^{(i)}(t)\frac{\partial}{\partial x}\phi_g^{(i)}. \tag{7}$$

This way, we need to introduce auxiliary equations to solve this problem. Then, we propose to approximate the current densities as a function of the average neutron fluxes based on study presented in REF. [5]. In this way, we write the current densities at the interfaces of node (i) as

$$J_g^{(i)}(x_i,t) \simeq -\frac{2\left(D_g^{(i+1)}(t)\Delta x^{(i+1)} + D_g^{(i)}(t)\Delta x^{(i)}\right)}{(\Delta x^{(i+1)} + \Delta x^{(i)})^2}\left(\underline{\phi}_g^{(i+1)}(t) - \underline{\phi}_g^{(i)}(t)\right) \tag{8}$$

and

$$J_g^{(i)}(x_{i-1},t) \simeq -\frac{2\left(D_g^{(i)}(t)\Delta x^{(i)} + D_g^{(i-1)}(t)\Delta x^{(i-1)}\right)}{(\Delta x^{(i)} + \Delta x^{(i-1)})^2}\left(\underline{\phi}_g^{(i)}(t) - \underline{\phi}_g^{(i-1)}(t)\right). \tag{9}$$

Ultimately, when we substitute the approximations of the current densities, we obtain a differential equations system in the temporal variable. For details see REF. [5].

2.2. Time variable

In this subsection, we propose to approach the time-dependent differential equations system in two decoupled subsystems: one for the neutron fluxes equations and the other for the delayed neutron precursor concentrations equations. Furthermore, an iterative process

between the two subsystems is applied. This treatment is necessary due to the presence of precursor concentrations in the source terms of neutron fluxes equations and conversely. In this way, we consider two subsystems in the form

$$\frac{d}{dt}\underline{\zeta}_p^{[s]}(t) = -\lambda_p \underline{\zeta}_p^{[s]}(t) + \beta_p S_{pre}^{[s-1]}(t) \tag{10}$$

and

$$\frac{d}{dt}\underline{\Phi}^{[s]}(t) = VM(t)\underline{\Phi}^{[s]}(t) + VS_{flu}^{[s]}(t), \tag{11}$$

where $\underline{\zeta}_p^{[s]}(t)$ is the $N \times 1$ vector of the average precursor concentration of the family p. $S_{pre}(t)$ is the $N \times 1$ source vector of the delayed neutron precursor concentration equations, where each component is defined as

$$\sum_{g=1}^{G} \nu_g \Sigma_g^{(i)} \underline{\phi}_g^{(i)}(t)\,. \tag{12}$$

Furthermore, V is the $NG \times NG$ blocks diagonal matrix, which contains the neutron velocities, $\underline{\phi}(t)$ is $GN \times 1$ vector of the average neutron fluxes. $M(t)$ is a $NG \times NG$ matrix with five diagonal blocks and $S_{flu}(t)$ is the $GN \times 1$ vector source vector for the differential subsystem of neutron fluxes, where each component is defined as

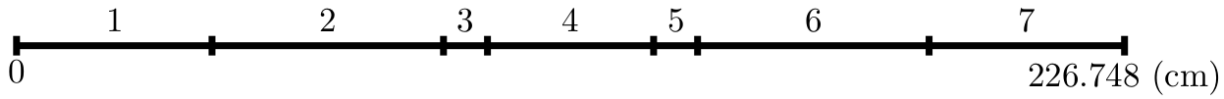
$$\chi_g^d \sum_{p=1}^{P} \lambda_p \underline{C}_p^{(i)}(t)\,. \tag{13}$$

The REF. [5] presents the detailed derivation and a comparative study between different forms of solution for the Eqs. (10) and (11). This study concluded that in most cases analytical treatment with constant sources for Eq. (10) and numerical treatment (Backward Euler method) for Eq. (11) is the best choice to get accurate results with low computational cost.

3. NUMERICAL RESULTS AND DISCUSSIONS

In this section, the motivation is to verify the influence of the diffusion approximation in global calculations in reactor physics. For this, we make a comparison between the numerical results obtained through the theory of neutron transport and the theory of neutron diffusion for the problems of criticality and spatial kinetics. In this context, we investigate Test Problem 16-A1, REF. [6], which is a problem defined in a medium with isotropic scattering and azimuthal symmetry, which consists of a heterogeneous medium with seven regions as shown in Figure 1 and Table 1.

Figure 1: Geometry of the Test Problem 16-A1.



Together with the dimensions of the seven regions, in Table 1, we present a proposal for the subdivision of each region, as presented by REF. [6]. This subdivision aims to establish an initial pattern for the mesh generation.

Table 1 : Test Problem 16-A1 spatial domain.

Region	Dimension (cm)	Node numbers
1	40	20
2	47.374	24
3	9	5
4	34	16
5	9	5
6	47.374	24
7	40	20

Source : American Nuclear Society (1985) [6].

Regions 1 and 7 are composed from the same coating material (Material 1), Regions 2, 4 and 6 are composed from the same combustible material (Material 2) and Regions 3 and

5 are a mixture of sodium and the material from the bars control (Material 3). The core parameters of each material are described in Table 2.

Table 2 : Parameters of Test Problem 16-A1.

Material	g	$\nu_g\Sigma_{fg}(cm^{-1})$	$\Sigma_{tg}(cm^{-1})$	$\Sigma_{sgg}(cm^{-1})$	$\Sigma_{sgg'}(cm^{-1})$
1	1	8.34410×10^{-4}	2.4110×10^{-1}	2.33644×10^{-1}	3.5980×10^{-3}
1	2	3.27760×10^{-4}	4.1720×10^{-1}	4.07004×10^{-1}	0.0
2	1	7.45180×10^{-3}	1.8490×10^{-1}	1.77711×10^{-1}	2.0850×10^{-3}
2	2	1.10612×10^{-2}	3.6680×10^{-1}	3.53721×10^{-1}	0.0
3	1	0.0	9.4320×10^{-2}	8.57100×10^{-2}	1.7168×10^{-3}
3	2	0.0	1.8762×10^{-1}	1.71310×10^{-1}	0.0
χ_1 =1.0	χ_2 =0.0				

Source: American Nuclear Society (1985) [6].

Table 2 presents the macroscopic cross-sections used in the neutron transport theory, however, to apply them in the diffusion theory we need the diffusion coefficients. Since this is an isotropic scattering problem, we define the diffusion coefficient as

$$D_g = \frac{1}{3\Sigma_{tg}} \ . \tag{14}$$

In addition, we also need the removal cross-section, determined in the form

$$\Sigma_{Rg} = \Sigma_{tg} - \Sigma_{sgg} \ . \tag{15}$$

3.1. Steady state problem

Our results for the K dominant eigenvalue in the steady state problem are generated by the Secant method proposed in REF. [7], in addition to the approximations of the current densities at the interfaces that we introduced in Section 2.1 in this work. The results via neutron transport theory that we adopted for comparison are those presented in REF. [6],

which was provided by the Argonne National Laboratory. Paragraph 16-A1 Problem Test, REF. [6] presents the results obtained through two codes:

- 16-A1-1 (TIMEX code) obtained K = 1.000198
- 16-A1-2 (TDA code) obtained K = 1.000000

where the TDA code treats the values of the scalar fluxes as average values of the mesh interval and the TIMEX code values in the limits of the mesh intervals.

For comparison purposes, we also adopted the dominant eigenvalues calculated using the diffusion equation by REF. [8]. Even though his thesis is more specifically for transport problems, he presents some results based on diffusion. Banfield proposes a semi-implicit direct kinetics (SIDK) method developed for the neutron transport equation. This method is a modification of the diffusion kinetics method developed by REF. [9]. In REF. [8] says that the only differences in the derivation are that the scattering term is included in the leakage operator and that the derivation is done for a generic number of energy groups. Therefore, as it does not show how spatial discretization is performed, we believe that it is the same as REF. [9], which is based on the Legendre polynomial expansion.

Table 3 : Results for the dominant eigenvalue K for Test Problem 16-A1 via diffusion.

Node	REF. [8]			Secant method [7]		
numbers	K	error Timex	error TDA	K	error Timex	error TDA
114	0.991826	0.00837	0.00817	0.99389	0.00631	0.00611
228	0.992923	0.00727	0.00708	0.99385	0.00635	0.00615
456	0.993431	0.00677	0.00657	0.99390	0.00630	0.00610
912	0.993675	0.00652	0.00633	0.99394	0.00626	0.00606

The first aspect that we highlight in Table 3 is the difference in the state of criticality obtained via transport and via diffusion. In transport, the result obtained by the TIMEX

code indicated a core in a supercritical state (K = 1.000198) and the TDA code a critical state (K = 1.000000). However, in diffusion, the results indicate a subcritical state, both in REF. [8] and in our results. When we take the results obtained via transport as a reference, we observe that our methodology produced closer results (lower relative errors) than the Banfield results. Finally, when comparing the results obtained via diffusion, we noticed an agreement of up to three significant digits, however, for the meshes presented, our results set one digit more than REF. [8].

The graphs in Figures 2 and 3 bring a comparison between the scalar fluxes determined by the transport theory and by the diffusion theory. As we work with average scalar flux, we adopted as reference the fluxes obtained by the TDA code [6]. Diffusion graphs are obtained with a mesh of 912 nodes.

Figure 2: Illustration of the average fast neutron fluxes of Test Problem 16-A1.

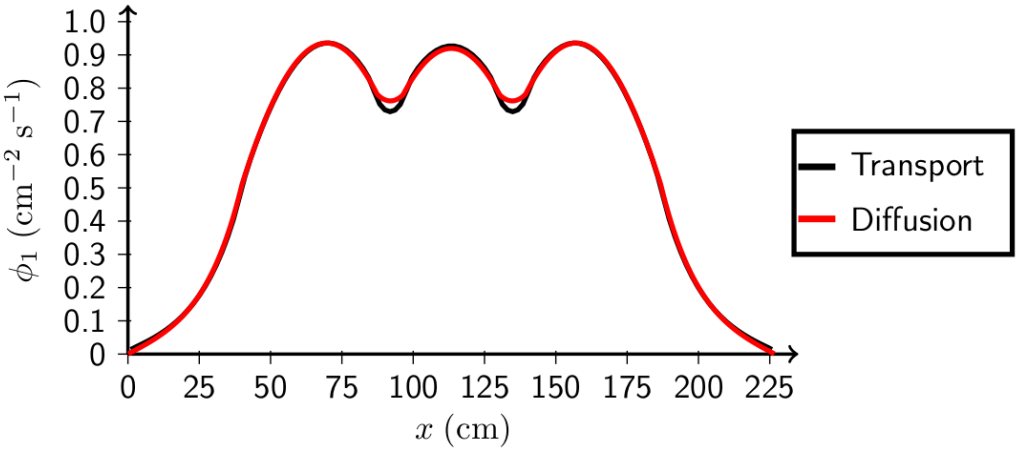
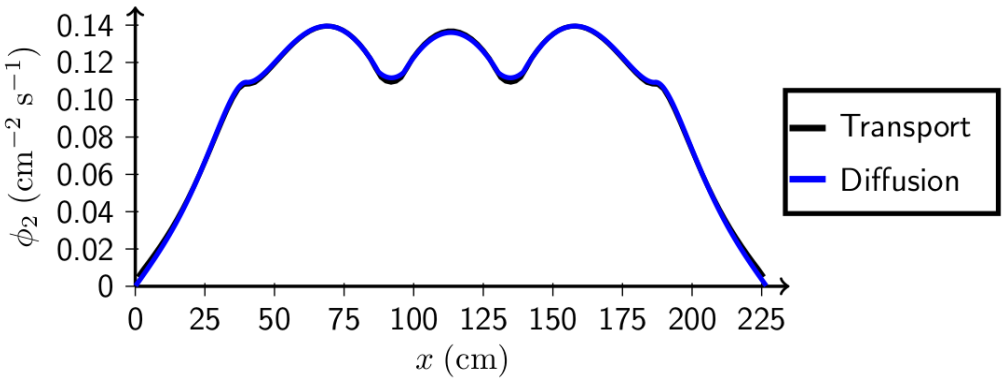


Figure 3: Illustration of the average thermal neutron fluxes of Test Problem 16-A1.



In Figures 4 and 5, we present the error between the fluxes determined by transport and diffusion. For a better visualization, in the figures we added the limits of each material region. The absolute error is determined by subtracting the results for transport-determined fluxes by the diffusion determined fluxes.

Figure 4: Illustration of the absolute error of average fast neutron fluxes of Test Problem 16-A1.

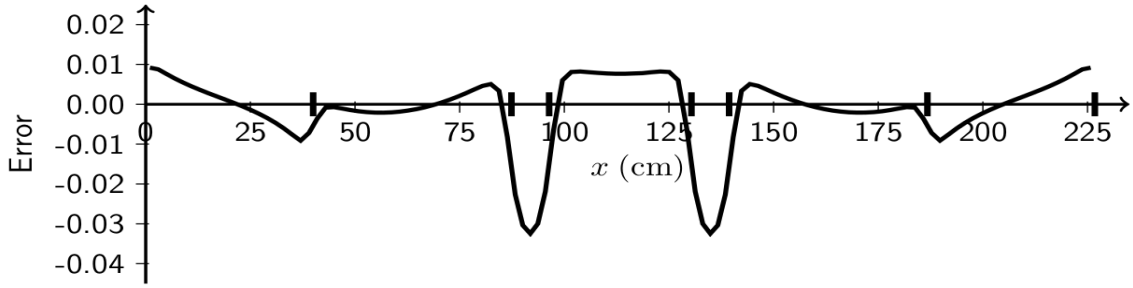
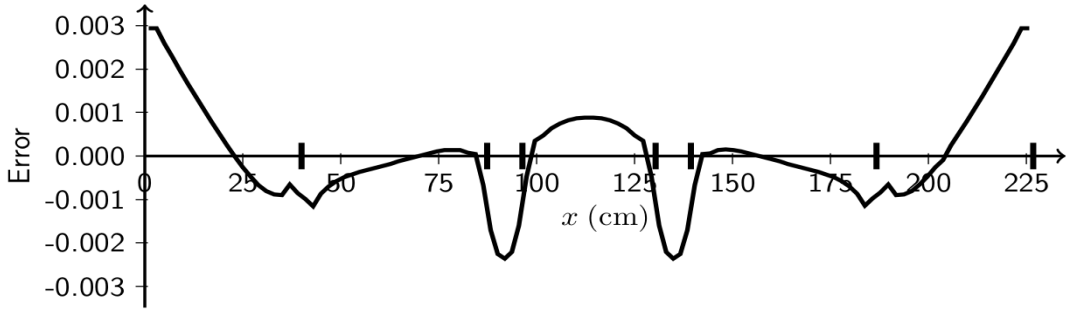


Figure 5: Illustration of the absolute error of average thermal neutron fluxes of Test Problem 16-A1.



In Figures 4 and 5, the error presented by the diffusion approximation was observed, in particular in the limits of the materials and in the strongly absorbing materials (Regions 3 and 5).

3.2. Spatial kinetics problem

The Test Problem 16-A1 of ANL Benchmark is a one-dimensional fast reactor benchmark. This is an excellent problem to examine the impact of transport versus diffusion solutions, as it is one of the few transport-based spatial kinetics benchmarks available in the literature [8].

At time t = 0s, an instantaneous disturbance is made to the densities of the materials in Regions 2 and 6. The change consists of a 5% increase in density in Region 2 and a 5% decrease in Region 6, that is, a change in the number of nuclei per unit volume. This perturbation results in a change in the cross-sections of Regions 2 and 6 in Table 2. We present the other parameters for the kinetic problem in Table 4.

Table 4 : Parameters for kinetic of Test Problem 16-A1.

i	β_i	λ_i	χ_i^d	v_i
1	0.810×10^{-4}	0.0129	1.0	$10^9/1.851$
2	6.870×10^{-4}	0.0311	0.0	$10^8/1.088$
3	6.120×10^{-4}	0.1340		
4	1.138×10^{-3}	0.3310		
5	5.120×10^{-4}	1.2600		
6	1.700×10^{-4}	3.2100		

Source : American Nuclear Society (1985) [6].

In Figures 6 and 7, the graphs refer to the SIDK method in REF. [8] were extracted from the figures presented by the author through the App WebPlotDigitizer. On the other hand, the graphs refer to the solution via transport (TDA code) are obtained by plotting the tabulated results presented in REF. [6].

Figure 6: Illustration of the average fast neutron fluxes of Test Problem 16-A1.

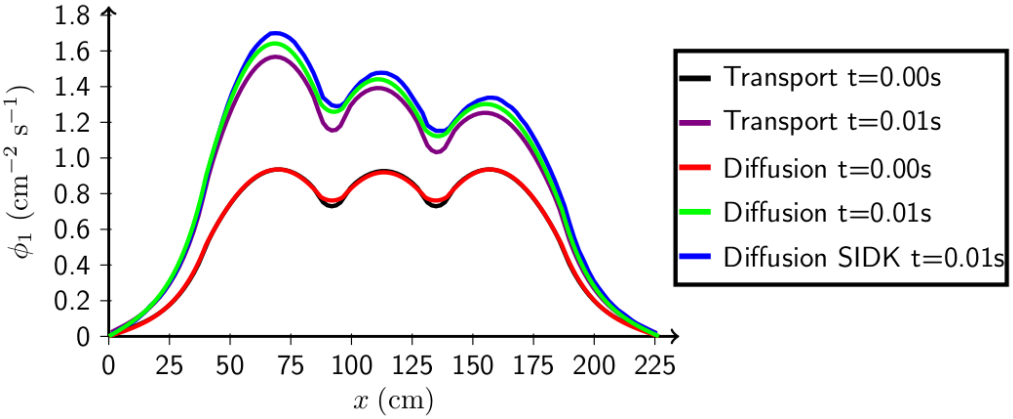
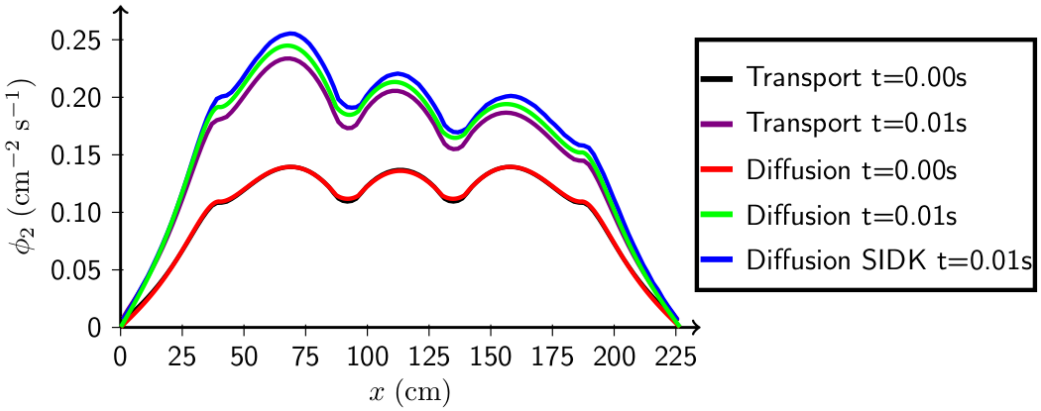


Figure 7: Illustration of the average thermal neutron fluxes of Test Problem 16-A1.



In the graphs in Figures 6 and 7 we notice that both results (ours and REF. [8]) obtained via diffusion theory have a small upward variation in relation to the results obtained via transport theory. Furthermore, we observed that our results for the fluxes at t = 0.01s are in better agreement with the ones to the fluxes obtained by the transport theory than the fluxes obtained by REF. [8].

In Table 5, we present a comparison between the flux values obtained via transport and via diffusion, in addition with the relative error. When observing the column of relative errors, we noticed that the biggest errors are found in the nodes that make limits with the contours. This behavior was already expected since this is one of the places where the

diffusion approximation is not satisfactory due to Fick's Law. In the other nodes, we obtained small relative errors, in the order of 10^{-2}.

Table 5 : Comparison of the scalar fluxes of Test Problem 16-A1 in time 0.01s.

Node	ϕ_1^{Trans}	ϕ_1^{Diff}	Rel. error	ϕ_2^{Trans}	ϕ_2^{Diff}	Rel. error
1	0.02294	0.00795	0. 65334	0.00843	0.00368	0.56374
10	0.19025	0.19722	0.03668	0.07894	0.08179	0.03607
20	0.78486	0.83469	0.06348	0.18007	0.19105	0.06098
30	1.47690	1.55075	0.05001	0.22399	0.23508	0.04952
40	1.48072	1.54348	0.04238	0.21884	0.22873	0.04520
50	1.23444	1.30073	0.05370	0.18239	0.19139	0.04938
60	1.34930	1.39520	0.03402	0.19914	0.20643	0.03660
70	1.05702	1.13393	0.07276	0.15763	0.16665	0.05723
80	1.24768	1.29737	0.03983	0.18633	0.19380	0.04008
90	0.95046	0.98964	0.04123	0.15620	0.16318	0.04470
100	0.31208	0.32912	0.05461	0.10817	0.11335	0.04788
110	0.06540	0.06044	0.07578	0.02893	0.02732	0.05557
114	0.01836	0.00631	0.65603	0.00674	0.00292	0.56713

4. CONCLUSIONS

The transport equation that could predict the neutron distribution in detail for the design of nuclear reactors is still a challenge to be solved in its complete form. The diffusion equation is commonly used as a simpler model generating good results. In this work, we established a comparison of the two models in order to analyze the results for the K dominant eigenvalue and scalar fluxes.

Comparing the two theories, in the particular case chosen in this study, especially in the interface regions and near the boundaries, the results found aligned with what was expected by theory, and it was possible to establish a more accurate absolute percentage error of the actual difference between the theories.

Possible modifications of neutron diffusion theory would be welcome in the sense of reducing the error concerning the more comprehensive model of neutron transport theory. Although a potential source of error in diffusion theory, namely Fick's Law, is widely acknowledged, quantitative results in this magnitude are not as firmly established, especially when the assumptions of its validity are not met. To find a new closure model that yields results closer to transport theory than the classical one, numerical results need to be established in depth, particularly in regions of significant neutron population variation where the validity of the law is not appropriate, in order to establish possible modifications to Fick's Law.

Theoretical developments in this direction are already underway. Therefore, the contributions of this work have enabled the production not only of a computational tool that can be effectively used to generate results that constitute a good mathematical benchmark for testing numerical algorithms and codes to be adopted for reactor physics evaluations but also to produce a preliminary discussion on a new model to be adopted for the kinetics equations in order to increasingly approximate the realistic transport solution.

ACKNOWLEDGMENT

This research was supported by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and the Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul (FAPERGS).

FUNDING

This study was financed in part by the Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) - Brasil, the Coordenação de Aperfeiçoamento de Pessoal

de Nível Superior (CAPES) - Brasil (Finance Code 001) and the Fundação de Amparo à Pesquisa do Estado do Rio Grande do Sul (FAPERGS): (Proc: 19/2551-0001766-9).

CONFLICT OF INTEREST

All authors declare that they have no conflicts of interest.

REFERENCES

[1] BELL, G. I.; GLASSTONE, S. **Nuclear Reactor Theory**. 1th ed. Van Nostrand Reinhold Company, 1970.

[2] DUDERSTADT, J. J.; HAMILTON L. J. **Nuclear reactor analysis**. New York: John Wiley, 1976.

[3] LEWIS, E. E. **Fundamentals of Nuclear Reactor Physic**. Elsevier Inc., 2008.

[4] GANAPOL, B. D. **Analytical Benchmarks for Nuclear Engineering Applications Case Studies in Neutron Transport Theory**. Paris: OECD Publishing, 2008.

[5] ZANETTE, R.; BARICHELLO, L. B.; PETERSEN, C. Z. A study on the solution of the spatial kinetics equations in the neutron diffusion theory. **Progress in Nuclear Energy**, v. 145, p. 104113, 2022.

[6] AMERICAN NUCLEAR SOCIETY. **National Energy Software Center: Benchmark problem book**. Illinois: ANL-7416, Supplement 3, 1985.

[7] ZANETTE, R.; BARICHELLO, L. B.; PETERSEN, C. Z. Cálculo de criticalidade pela teoria de difusão de nêutrons: uma análise comparativa de aproximação da densidade de corrente. **REMAT: Revista Eletrônica da Matemática**, v. 6, n. 2, p. e4006, 2020.

[8] BANFIELD, J. E. **Semi-Implicit Direct Kinetics Methodology for Deterministic, Time-Dependent, Three-Dimensional, and Fine-Energy Neutron Transport Solutions.** PhD diss., University of Tennessee, 2013.

[9] GINESTAR, D.; VERDÚ, G; VIDAL, V.; BRU, R.; MARÍN, J.; MUÑOZ-COBO, J. L. High order backward discretization of the neutron diffusion equation. **Annals of Nuclear Energy**, v. 25, p. 47–64, 1998.

LICENSE