

Thermal Diffusion Properties of Moderating Materials H₂O and D₂O in Thermal Nuclear Reactors

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Abstract - Using techniques method of lines (MOL) and finite difference (FD) methods to solve the neutron diffusion equations (NDE). In this work, a new strategy was proposed to compute the neutron flux, concentration, and temperature properties of thermal nuclear reactors. This approach holds the potential for developing the static diffusion equation for different grades of temperature. Finite difference method was used to convert the parabolic partial differential equations into ordinary differential ones. The converted equations were generalized to consider three different geometries namely: spherical, cylindrical, and Cartesian. Moreover, MOL was used to solve the time-dependent NDE with space-time terms which describe the dynamics of one and two-groups. Results of the study showed that the thermal diffusion properties of moderating materials for H₂O found that the diffusion coefficient (D), diffusion length (L) and Albedo $\beta(\infty)$ were 0.142 cm, 2.88 cm, and 0.82, respectively. While the same diffusion properties for heavy water (D₂O) were D=0.8 cm, L=100.0 cm, and $\beta(\infty)$ =0.968. Meanwhile, D=0.903 cm, L=50.0 cm, and $\beta(\infty)$ =0.930 for Graphite (14C). The generated results are compatible with other different methods of calculations. This study recommends using the MOL to solve the NDE as it gives more accurate results and practically efficient for thermal neutron reactors.

Keywords: Neutron diffusion equations, Method of lines, Finite difference methods, Neutron flux, Thermal nuclear reactors.

I. INTRODUCTION

The neutron diffusion equation (NDE) is a basic balance equation that describes the transport of neutrons in space, energy, and time. This equation plays a central role in reactor physics, because the NDE solution provides the neutron flux, which is required to represent the rate at which neutrons interact with the surrounding medium and the rate at which they leak out of a given volume [1,2]. NDE describes the density of neutrons in a nuclear reactor core. Scientists and engineers have been working for many years to develop

accurate approaches to analyzing nuclear power reactors using computer codes that closely model the behavior of neutrons in a reactor core [3]. Many calculation methods have been proposed to solve diffuse neutron mostly based on the method of finite difference (FD) applied to the domain geometric shape such as in the case of Cartesians, spherical and cylindrical coordinates [4,5]. The nuclear reactor problems, especially those involving safety considerations, the coefficients of the neutron diffusion equations depend upon parameters such as the neutron power level, precursor concentration of delayed neutrons groups, time, space and temperature feedback [6-9].

The nuclear reactor is a complex fuel system competition, with reflectors, coolants, control rods and other parts. The design and analysis of such reactors for different operating methods is part of a complex task involving several disciplines of nuclear engineering. Among the most important is the determination of neutron flux distribution within the reactor core and finding the critical dimension and mass. This issue has received considerable attention in the field of reactor physics in the past decades [10,11]. In general, the reactor problem in the presence of Newtonian temperature feedback effects comprises a very large and complex system of coupled nonlinear partial differential equations. Numerical methods for solving the space-time neutron diffusion equations in the nuclear reactor have been of interest in the nuclear reactor physics and engineering [6,12]. An efficient solution method was presented to solve the time-dependent multi-group diffusion equations for the subcritical systems with external sources using a rigorous weight function in the quasi-static method.

During the last few decades, some authors have used the hybrid method between a method and a method of other groups to take advantage of these methods simultaneously overcoming the disadvantages and shortcomings of each method. The mixed dual nodal method was used to solve the reactor kinetics equations with improved quasi-static model and the θ -method was used to solve the precursor equations [6,13]. An efficient solution method was presented to solve the time-dependent multi-group diffusion equations for the

subcritical systems with external sources using a rigorous weight function in the quasi-static method [14]. Parallelized Krylov methods were applied to improved quasi-static approach in addition to the direct, implicit time difference, approach for solving space-time dependent multi-group neutron diffusion equations [15,16]. The nodal diffusion method was developed to solve space-time neutron kinetics using the finite-element, primal and mixed hybrid nodal methods [17]. A one-step implicit method and a nodal modal method were studied to solve the time dependent neutron diffusion equations which are based on a hexagonal spatial mesh [18,19]. Numerical technique, based on the class of Padre and cut-product approximations, was applied to solve the two-energy group space-time nuclear reactor kinetics equations in two dimensions [16]. The generalized Runge-Kutta method was developed for solving the multi-group, multidimensional, static and transient neutron diffusion kinetics equations [20]. Computation accuracy and efficiency of a power series analytic method were presented for the time-space dependent neutron diffusion equations with adiabatic heat up and Doppler feedback [21].

In this work, numerical methods of lines (MOL) for space-time neutron diffusion equations with multi-groups of thermal nuclear reactors are developed. The partial differential equations are changed to ordinary differential equations using the finite difference method. The matrix form of ordinary differential equations is obtained. Neutron diffusion equations are solved in several cases and neutron diffusion in a Cartesian coordinate with mixed boundary conditions are presented. Both neutron concentration and temperature flow are calculated to find a steady-state of one-energy group of NDE in spherical and cylindrical thermal reactors. The analytical method and fundamental matrix method for the exponential function of the coefficient matrix are presented. The results of numerical MOL are discussed and compared with the results of analytical methods.

II. THEORETICAL FRAMEWORK

2.1 Multi-group neutron diffusion equation

The multi-energy group nuclear reactor kinetics equations with multi-group delayed precursor neutrons can be written in the following form [1,2,22-25].

$$\frac{1}{v_g} \frac{\partial}{\partial t} \Phi_g(r, t) = \nabla \cdot D_g(r) \nabla \Phi_g(r, t) - \Sigma_{a_g} \Phi_g(r, t) - \sum_{g' > g} \Sigma_{s_{g,g'}} \Phi_{g'}(r, t) + \sum_{g'=1}^G (\chi_g v \Sigma_{f_{g'}} (1 - \beta) + \Sigma_{s_{g,g'}} \Phi_{g'}(r, t) + \sum_{i=1}^I \lambda_i C_i(r, t)) \quad (1)$$

$$\frac{\partial}{\partial t} C_i(r, t) = \beta_i \sum_{g=1}^G v \Sigma_{f_g} \Phi_g(r, t) - \lambda_i C_i(r, t), \quad i = 1, 2, \dots, I \quad (2)$$

where: r is the position vector in (cm), t is the time (s), $\Phi_g(r, t)$ is the scalar neutron flux ($\text{cm}^{-2}\text{s}^{-1}$) in group g , $C_i(r, t)$ is the concentration of delayed neutron precursors (cm^{-3}) in group i . v_g is the mean velocity of the neutron (cm s^{-1}) in group g , $D_g(r)$ is the diffusion coefficient (cm) in group g . $\Sigma_{a_g}(r, t)$ is the absorption cross-section (cm^{-1}) in group g , $\Sigma_{f_g}(r)$ is the fission cross-section (cm^{-1}) in group g . $\Sigma_{s_{g,g'}}(r)$ is the scattering cross-section (cm^{-1}) from group g' to group g such that $(\Sigma_{s_{g',g}}(r) = 0 \text{ for } g' > g)$, ν is the mean number of fission neutrons. χ_g is the spectrum of prompt neutrons in group g , $\chi_{g,i}$ is the spectrum of i -group delayed neutrons in group g , λ_i is the decay constant (s^{-1}) of group i precursors. β_i is the fraction of delayed neutrons in group i , and $\beta = \sum_{i=1}^I \beta_i$ is the total fraction of delayed neutrons. Using the finite difference method (FDM), the equations (1) and (2) lead to the following matrix form [26-29].

$$\frac{d\Psi(t)}{dt} = A\Psi(t) + B \quad (3)$$

where the wave function $\Psi(t)$, and matrices A and B are defined with all the coefficients in Refs [32-35]. Assume that the matrices A and B are constant during the interval time t_m and $t_{m+1} = t_m + h$ considering the length of the time interval is small. Then, the general analytical solution of Eq. (3) with A and B constant, is

$$\Psi(t_{m+1}) = \exp(hA)\Psi(t_m) + (\exp(hA) - I)A^{-1}B \quad (4)$$

There are several numerical techniques for calculating the exponential function of the coefficient matrix A [30]. The aim of the study is to find the simple solutions of steady-state neutron diffusion equation (1) in non-multiplying media to illustrate the basic approach we take for the solution including the application of boundary conditions. We begin with solutions in simple geometries, subject to localized source distribution, which are idealized as simplifying the necessary mathematical steps.

III. COMPUTATIONAL METHODS

3.1 One-dimensional neutron diffusion equation

The partial differential equation (PDE) problem is the one-dimensional heat conduction equation in cartesian coordinates[1,2,22-25].

$$u_t = Du_{xx} \tag{5}$$

Here, we have used subscript notation for partial derivatives, so $u_t \leftrightarrow \partial u / \partial t$ and $u_{xx} \leftrightarrow \partial^2 u / \partial x^2$.

The initial condition (IC) is: $u(x, t = 0) = \sin(\pi x / 2)$ (6)

A Dirichlet boundary condition (BC) is specified

$$\text{at } x = 0, \quad u(x = 0, t) = 0 \tag{7}$$

And a Neumann BC is specified at $x = 1, u_x(x = 1, t) = 0$ (8)

The analytical solution to Eqs. (6)-(8) is:

$$u(x, t) = e^{-(\pi^2/4)t} \sin(\pi x / 2) \tag{9}$$

A main program in MATLAB for the MOL solution of Eqs. (5)-(8) with the analytical solution, Eq. (9), will be included for comparison with the MOL solution [24,31-33]. We noted the following points about the main program used: (1) After declaring some parameters global so that they can be shared with routines called via this main program, IC (6) is computed over a 21-point grid in x , (2) The independent variable t is defined over the interval $0 \leq t \leq 2.5$; again, a 21-point grid is used, and (3) the 21 ordinary differential equations (ODEs) are integrated by a call to the MATLAB integrator ode15s.

3.2 Initial and boundary conditions

Before considering a solution to Eq. (3.1), one must specify some auxiliary conditions to complete the statement of the NDE problem. The number of required auxiliary conditions is determined by the highest-order derivative in each independent variable. Since Eq. (3.1) is first order in t and second order in x , it requires one auxiliary condition in t and two auxiliary conditions in x . To have a complete, well-posed problem, some additional conditions may have to be included, for example, that specify valid ranges for coefficients. However, this is a more advanced topic and will not be developed further here.

t is termed an initial-value variable and therefore requires one initial condition (IC). It is an initial-value variable since it starts at an initial value, t_0 , and moves forward over a finite interval $t_0 \leq t \leq t_f$ or a semi-infinite interval $t_0 \leq t \leq \infty$ without any additional conditions being imposed. Typically, in a NDE application, the initial-value variable is time, as in the case of Eq. (1). x is termed a boundary-value variable and therefore requires two boundary conditions (BCs). It is a boundary-value variable since it varies over a finite interval $x_0 \leq x \leq x_f$, a semi-infinite

interval $x_0 \leq x \leq \infty$, or a fully infinite interval $-\infty \leq x \leq \infty$, and at two different values of x , conditions are imposed on u in Eq. (4). Typically, the two values of x correspond to boundaries of a physical system, and hence the name boundary conditions. An IC could be $u(x, t = 0) = u_0$ and two BCs could be $u(x = 0, t) = u_b$, $u_x(x = x_f, t) = 0$, where u_b is a given boundary (constant) of u for all t .

3.3 Numerical solutions of neutron diffusion equation

The computer-based numerical solution of the partial differential equations (PDEs), such as NDE models is implemented primarily through the method of lines (MOL). Therefore, we start with this subsection, which is a basic idea to the MOL for PDE. Although the reader may be familiar with MOL, one suggests reading this subsection since it describes some aspects and details of our use of the MOL [25]. The physical world is most generally described in scientific and engineering terms with respect to three-dimensional (3D) space and time, which we abbreviate as space-time. NDEs provide a mathematical description of physical space-time, and they are therefore among the most widely used forms of mathematics. Consequently, methods for the solution of PDEs, such as the MOL, are of broad interest in science and engineering. As a basic illustrative example of a PDE, we consider Eq. (1) where function $u(x, t)$ dependent variable on x and t . Equation (1) is termed the neutron diffusion equation (NDE). When applied to NDE heat transfer, it is Fourier's second law; the dependent variable u is temperature and D is the thermal diffusivity. When Eq. (1) is applied to mass diffusion, it is Fick's second law; u is mass concentration and D is the coefficient of diffusion or the diffusivity.

IV. RESULTS AND DISCUSSIONS

In this section we show the numerical results and the comparison with analytical solutions of NDE descriptions of nuclear reactors. The output displayed in table 1 indicates that the MOL solution agrees with the analytical solution to at least three significant figures.

Table 1: Output for mf=1, abstol=1.0e-004 and ncall=85 from pde-main

time (t)	numerical u(0.5,t)	analytical u(0.5, t)	error u(0.5, t)
0.000	0.707107	0.707107	0.0000000
0.625	0.151387	0.151268	0.0001182
1.250	0.032370	0.032360	0.0000093
1.875	0.006894	0.006923	-0.0000283
2.500	0.001472	0.001481	-0.0000091

The plotted error output shown in Figure 1 indicates that the error in the MOL solution varied between approximately

-3×10^{-5} and 16×10^{-5} , which is not quite within the error range specified in the program. The fact the error tolerances illustrated in Figure 1 were not satisfied does not necessarily mean that ode15s failed to adjust the integration interval to meet these error tolerances. Rather, the error of approximately 1.6×10^{-4} is due to the limited accuracy of the second-order FD approximation of $\partial^2 u / \partial x^2$ programmed in pde_1. This conclusion is confirmed when the main program call pde_2 (for mf=2) or pde_3 for mf=3), as discussed subsequently; these two routines have FD approximations that are more accurate than in pde_1, so the errors fall below the specified tolerances.

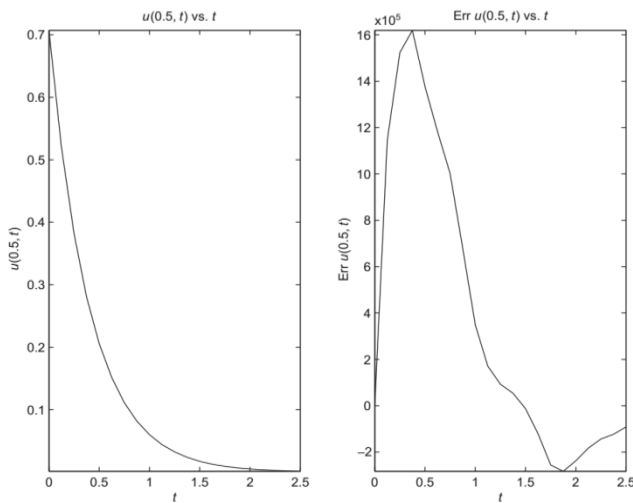


Figure 1: Showing two-dimensional graphical output from pde_1_1 main at mf=1

This analysis indicates that two sources of errors result from the MOL solution of PDEs such as Eq. (1): (a) errors due to the integration in t (by ode15s) and (b) error due to the approximation of the spatial derivatives such as $\partial^2 u / \partial x^2$ programmed in the derivative routine such as pde_1. In other words, we must be attentive to integration errors in the initial- and boundary-value independent variables [24]. A comparison of the numerical and analytical solutions indicates that 21 grid points in x were not sufficient when using the second-order FDs in pde_1. However, in general, we will not have an analytical solution such as Eq. (3.5) to determine if the number of spatial grid points is adequate. In this case, some experimentation with the number of grid points, and the observation of the resulting solutions to infer the degree of accuracy or spatial convergence, may be required as shown in figures (2-4).

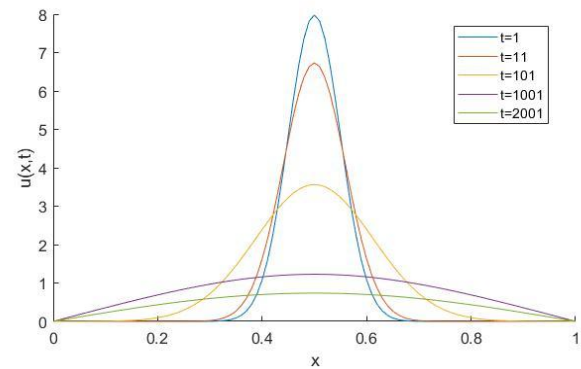


Figure 2: Show distributions solution of diffusion equation with constant concentration boundary conditions

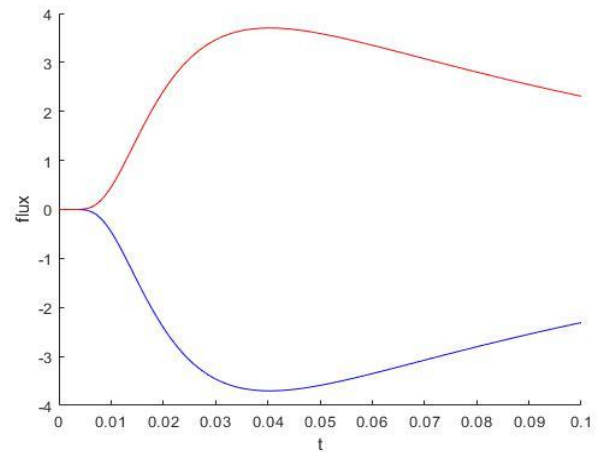


Figure 3: Show nuclear reactor flux at the boundaries $x=0$ (blue line) and $x=1$ (red line)

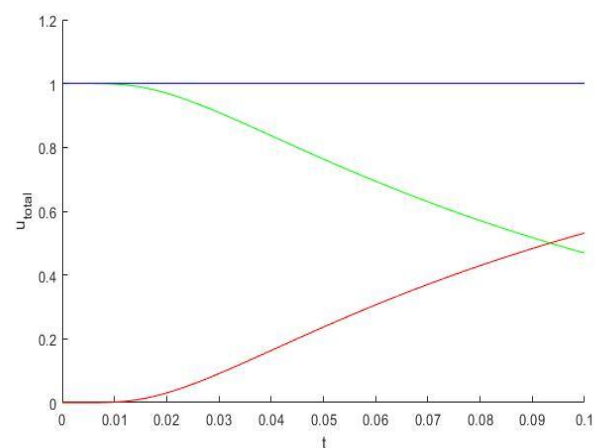


Figure 4: Total distributions functions u (green line), u_0+u_1 (red line) and $u+u_0+u_1$ (blue line) with time

Figure 5 show solution of single heat equation using boundary conditions.

$$p(x_i, t, u) + q(x_i, t). b(x_i, t, u, u_x) = 0$$

$$p(x_r, t, u) + q(x_r, t).b(x_r, t, u, u_x) = 0$$

where x_l represents the left endpoint of the boundary and x_r represents the right endpoint of the boundary, and the initial condition $u(0, x) = f(x)$. Observe that the same function b appears in both the equation and the boundary conditions.

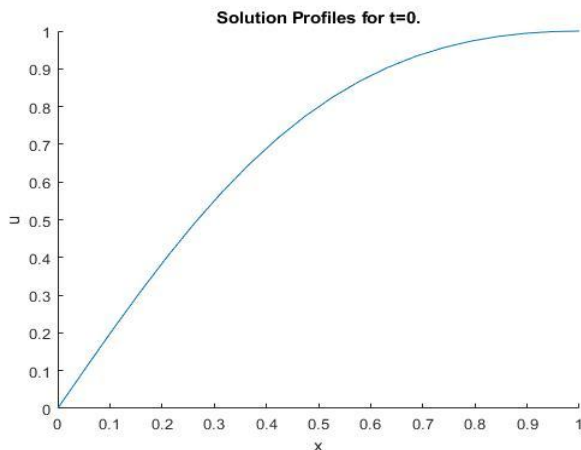


Figure 5: Distributions functionsvs space

Figures 6, 7 show numerical solution of 1D heat equation using FD and BD methods. Solving equation: $u_t = \beta u_{xx}$ with initial conditions $u_j^0 = f(x_j) = u(x, t = 0)$, Dirichlet boundary conditions at $x = 0: u(x = 0, t) = u_0^k = g_1(t_k)$ and Neumann boundary conditions at $x = a: \partial u(a, t)/\partial t = \partial u_{n+1}^k/\partial x = g_2(t_k)$. To solve using Neumann boundary condition we need an extra step:

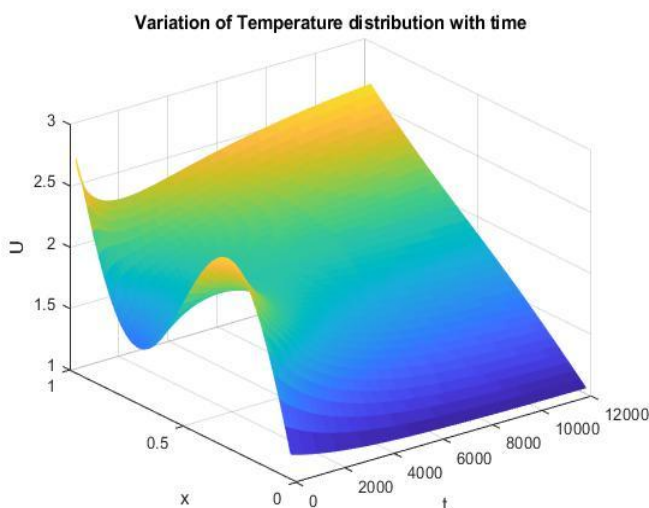


Figure 6: Variation of temperature distribution with time using forward Euler method

Variation of Temperature distribution with time using Backward Euler method

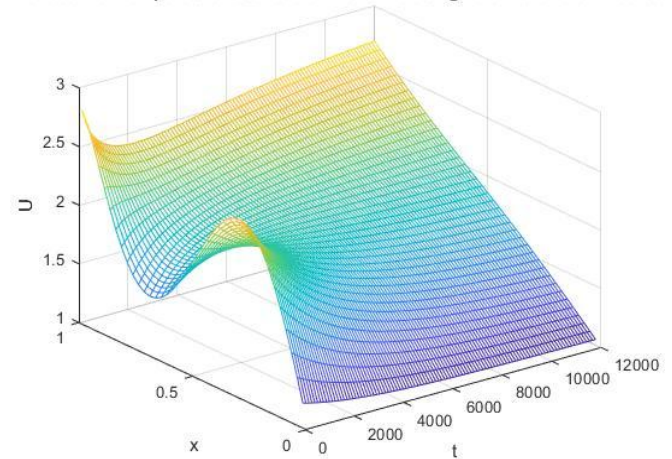


Figure 7: Variation of temperature distribution with time using backward Euler method

V. CONCLUSION

Numerical and analytical calculations based on finite difference (FD) method for neutron diffusion equation (NDE) in the thermal neutron reactor are considered. We use the method of line (MOL) to solve the NDE for complicated geometries. Combining MOL with FD method, we solve the NDE for the multigrain and one group for delayed neutrons in pressurized water reactor (PWR) core fuel. The solutions are expanded for all points in the 1D, 2D, and 3D mesh of the thermal reactor geometries. They are compared to other methods and analytical solution. In this study, combining MOL with FD method was used to solve the motion and interactions of neutrons inside a 1D, 2D, and 3D neutron in thermal reactor and calculated the neutron flux distribution for different times $u(x, t)$ are computed and compared between numerical solution and analytical solutions, therefore, found it for $t=0.625$ s, the flux density $u(0.5, t)=0.151387$ for numerical solution and $u(0.5, t)=0.151268$ for analytical solution, with error $u(0.5, t)=0.0001182$, and after long time $t=2.5$ s the flux density $u(0.5, t)=0.001472$ for numerical solution and $u(0.5, t)=0.001481$ for analytical solution, with error $u(0.5, t)=0.0000091$. In addition, calculated the flux distribution of NDE in 1D with constant concentration and boundary condition, it verified that the total flux distribution of neutron diffusion equation of thermal nuclear reactor is conserved

DATA AVAILABILITY STATEMENT

Data will be made available from the corresponding author on reasonable request.

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CONFLICT OF INTEREST

The study's authors confirm that no financial or commercial relationships that could create a conflict of interest occurred throughout their execution.

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