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ON THE EXACT SOLUTION FOR THE MULTI-GROUP KINETIC NEUTRON DIFFUSION EQUATION IN A RECTANGLE

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ABSTRACT

In this work we consider the two-group bi-dimensional kinetic neutron diffusion equation. The solution procedure formalism is general with respect to the number of energy groups, neutron precursor families and regions with different chemical compositions. The fast and thermal flux and the delayed neutron precursor yields are expanded in a truncated double series in terms of eigenfunctions that, upon insertion into the kinetic equation and upon taking moments, results in a first order linear differential matrix equation with source terms. We split the matrix appearing in the transformed problem into a sum of a diagonal matrix plus the matrix containing the remaining terms and recast the transformed problem into a form that can be solved in the spirit of Adomian's recursive decomposition formalism. Convergence of the solution is guaranteed by the Cardinal Interpolation Theorem. We give numerical simulations and comparisons with available results in the literature.

Key Words: Multi-Group Kinetics, Neutron Diffusion Equation, Benchmark Solution.

1. INTRODUCTION

In a recent work [1] the one dimensional kinetic neutron equation in a multi-layer slab was solved analytically by means of spectral theory [2, 3]. The multi-group formalism was implemented in its simplest form with two energy groups and six precursor yields for the delayed neutrons were considered. For problems of this type, one finds a vast literature predominantly based on numerical schemes for approximate solutions. To the best of our knowledge, no attempt has been published so far that focuses on an exact solution to the problem, except for analytical approaches [4–6].

In this work we extend the afore mentioned solution for the two-group bi-dimensional kinetic neutron diffusion equations. As we will show in the forthcoming discussion, the formalism is general in the sense that energy group extensions as well as multi-regions with different chemical compositions do not demand for modifications of the presented algorithm but increment only

the number of components of the equation system. Our formalism is constituted basically by the following steps. The fast and thermal flux as well as the delayed neutron precursor yields are expanded in a double series in terms of eigenfunctions, that solve exactly the one dimensional one-group problem. These series are inserted into the kinetic equations and, upon taking moments (projecting out orthogonal constituents of the equation), result in a first order linear differential matrix equation, known as the transformed problem. It must be born in mind that after orthogonal decomposition of the equations, the resulting matrices are of order $G \times N_1 \times N_2$, where G is the number of energy groups and N_1, N_2 are the number of terms of the double series summation, respectively.

If such an equation system is solved by standard techniques that make use of eigenfunctions and eigenvalues, the dimension of the equation system imposes computational limits. These difficulties are circumvented in this work following a reasoning inspired by the decomposition method [7]. We split the matrix appearing in the transformed problem into a sum of a diagonal matrix plus the matrix containing the remaining terms and recast the transformed problem as a matrix equation of the form: $\mathbf{X}' + \mathbf{DX} = -\mathbf{UX}$, where $\mathbf{D}$ is a diagonal matrix. The idea of the decomposition method [8] is to solve the linear matrix equation with source term as a closed form recursive process.

In the numerical applications of the solution, we complete our mathematical analysis discussing its convergence, using an analogy to the framework of the Cardinal Interpolation Theorem [9]. By this procedure we show that our solution is manifest exact and results can be evaluated to any prescribed precision by determining the necessary number of terms in the summation of the double series solution. We also report on numerical simulations and comparisons with available results in the literature and comment on the relevance of this solution.

The results obtained by the proposed technique can well constitute reliable benchmarks for the validation process of algorithms and numerical procedures.

2. A MANIFEST EXACT SOLUTION

In order to derive the exact solution for the multi-group kinetic neutron diffusion equations, in the following we restrict the analysis to a two energy-group model with six delayed neutron precursor families in a homogeneous rectangular domain, that imposes no restriction on generality, since the only change concerns the dimension of the matrix equation system:

$$\begin{aligned}
\frac{1}{v_1}\frac{\partial}{\partial t}\phi_1(x,y,t) &= D_1\left(\frac{\partial^2}{\partial x^2}\phi_1(x,t) + \frac{\partial^2}{\partial y^2}\phi_1(x,y,t)\right) - \Sigma_1\phi_1(x,y,t) \qquad (1)\\
&\quad +(1-\beta)\left(\nu_1\Sigma_{f1}\phi_1(x,y,t) + \nu_2\Sigma_{f2}\phi_2(x,y,t)\right) + \sum_{i=1}^{6}\lambda_i C_i(x,y,t)\ ,\\
\frac{1}{v_2}\frac{\partial}{\partial t}\phi_2(x,y,t) &= D_2\left(\frac{\partial^2}{\partial x^2}\phi_2(x,y,t) + \frac{\partial^2}{\partial y^2}\phi_2(x,y,t)\right) - \Sigma_2\phi_2(x,y,t) + \Sigma_{s12}\phi_1(x,y,t)\ , \qquad (2)\\
\frac{\partial}{\partial t}C_i(x,y,t) &= -\lambda_i C_i(x,y,t) + \beta_i\left(\nu_1\Sigma_{f1}\phi_1(x,y,t) + \nu_2\Sigma_{f2}\phi_2(x,y,t)\right)\ , \qquad (3)
\end{aligned}$$

where $i = 1, \ldots, 6$, for $t > 0$, $0 < x < L$ and $0 < y < M$. Here $\phi_1(x,y,t)$ and $\phi_2(x,y,t)$ indicate the fast and the thermal neutron flux, $C_i(x,y,t)$ is the delayed neutron precursor yield of family

i, v is the neutron velocity, D is the diffusion coefficient, Σ is the removal cross section, Σ_s is the scattering cross section, Σ_f is the fission cross section, ν is the average number of neutrons emitted per fission, β is the fraction of delayed neutrons and λ is the decay constant of the delayed neutron release process.

The system of equations (2-3) is subject to zero flux boundary conditions:

$$\phi(0,y,t) = \phi(L,y,t) = \phi(x,0,t) = \phi(x,M,t) = 0 \,, \tag{4}$$

and to initial conditions, assuming equilibrium delayed neutron precursors:

$$\begin{aligned} \phi_1(x,y,0) &= \phi_{1,0}(x,y) \,, \\ \phi_2(x,y,0) &= \phi_{2,0}(x,y) \,, \\ C_i(x,y,0) &= \frac{\beta_i \nu_1 \Sigma_{f1}}{\lambda_i}\phi_{1,0}(x,y) + \frac{\beta_i \nu_2 \Sigma_{f2}}{\lambda_i}\phi_{2,0}(x,y) \,, \end{aligned} \tag{5}$$

where $\phi_{1,0}(x,y)$ and $\phi_{2,0}(x,y)$ are the initial fast and thermal neutron fluxes at time $t = 0$.

In order to solve the equation system $(1-3)$ by the spectral method, introduced as GITT in refs. [2, 3], we add a spurious diffusion term in Eq. (3) for the precursor concentration, assuming also the homogeneous boundary condition, $C(0,y,t) = C(L,y,t) = C(x,0,t) = C(x,M,t) = 0$. This modification seems to be artificial and an unnecessary complication of the precursor equations, but fragments from fission in fact diffuse in the nuclear fuel, however with a vanishing diffusion constant. Furthermore, this inclusion allows to solve the combined system of neutron fluxes and precursor yields in one unique procedure. Hence, one can write:

$$\begin{aligned} \frac{\partial}{\partial t}C_i(x,y,t) &= \varepsilon\left(\frac{\partial^2}{\partial x^2}C_i(x,y,t) + \frac{\partial^2}{\partial y^2}C_i(x,y,t)\right) - \lambda_i C_i(x,y,t) + \beta_i \left(\nu_1 \Sigma_{f1}\phi_1(x,y,t)\right. \\ &\quad \left. + \nu_2 \Sigma_{f2}\phi_2(x,y,t)\right) \,, \end{aligned} \tag{6}$$

where $i = 1, \ldots, 6$ and ε is a positive small parameter. The above expansion and projection (i.e. the GITT method) may be applied to the equation, which in principle contains an infinite number of terms. At this point there is no need for a truncation and, in general, the expansion may be considered to run up to infinity for both summation indexes, which maintains the equation system exact. For practical purposes we already introduce the truncation indexes, which are usually used to compute numerical results, nevertheless we emphasize that the procedure for $N_1, N_2 \to \infty$ is exact. In this sense the exact solution is understood as the infinite limit and the formalism should be read, accordingly.

The neutron fluxes and delayed neutron precursor yields are:

$$\phi_1(x,y,t) = \sqrt{\frac{2}{L}}\sqrt{\frac{2}{M}}\sum_{m=1}^{N_2}\sum_{n=1}^{N_1}\phi_{1m,n}(t)\varphi_m(x)\psi_n(y) \,, \tag{7}$$

$$\phi_2(x,y,t) = \sqrt{\frac{2}{L}}\sqrt{\frac{2}{M}}\sum_{m=1}^{N_2}\sum_{n=1}^{N_1}\phi_{2m,n}(t)\varphi_m(x)\psi_n(y) \,, \tag{8}$$

$$C_i(x,y,t) = \sqrt{\frac{2}{L}}\sqrt{\frac{2}{M}}\sum_{m=1}^{N_2}\sum_{n=1}^{N_1}\xi_{im,n}(t)\varphi_m(x)\psi_n(y) \,, \tag{9}$$

where $i = 1, \ldots, 6$, $\varphi_m(x) = \sin(\lambda_m x)$ and $\psi_n(y) = \sin(\gamma_n y)$ are the eigenfunctions of the corresponding one-dimensional one group solution that may be interpreted as solution of an auxiliary Sturm-Liouville problem, constructed from the adjoint terms of the original problem, with eigenvalues λ_m and γ_n for each of the two-dimension degrees of freedom. Upon replacing this *ansatz* in the equation system (2-3), taking moments and projecting out orthogonal components collinear with one of the respective eigenfunctions, we end up with a matrix equation for the coefficients of the expansion:

$$\frac{d}{dt}\begin{pmatrix} \phi_{\mathbf{1m,n}}(\mathbf{t}) \\ \phi_{\mathbf{2m,n}}(\mathbf{t}) \\ \xi_{\mathbf{1m,n}}(\mathbf{t}) \\ \vdots \\ \xi_{\mathbf{6m,n}}(\mathbf{t}) \end{pmatrix} = -\begin{pmatrix} \mathbf{A} & \mathbf{B} & \mathbf{C_1} & \cdots & \mathbf{C_6} \\ \mathbf{F} & \mathbf{E} & \mathbf{Z} & \cdots & \mathbf{Z} \\ \mathbf{G_1} & \mathbf{H_1} & \mathbf{L_1} & \ldots & \mathbf{Z} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{G_6} & \mathbf{H_6} & \mathbf{Z} & \ldots & \mathbf{L_6} \end{pmatrix}\begin{pmatrix} \phi_{\mathbf{1m,n}}(\mathbf{t}) \\ \phi_{\mathbf{2m,n}}(\mathbf{t}) \\ \xi_{\mathbf{1m,n}}(\mathbf{t}) \\ \vdots \\ \xi_{\mathbf{6m,n}}(\mathbf{t}) \end{pmatrix} . \tag{10}$$

Here, $m = 1, \ldots, N_1$, $n = 1, \ldots, N_2$ and N_1 and N_2 are the truncation indexes for numerical calculations. Further, $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C_i}$, $\mathbf{F}$, $\mathbf{E}$, $\mathbf{G_i}$, $\mathbf{Z}$, $\mathbf{H_i}$ and $\mathbf{L_i}$ are diagonal $N_1 \times N_2$ matrices.

The first order homogeneous linear matrix equation in compact form is then:

$$\mathbf{X'(t)} + \mathbf{W}\,\mathbf{X(t)} = 0 \,, \tag{11}$$

with the well known solution

$$\mathbf{X(t)} = \exp(-\mathbf{W}\,t)\,\mathbf{X(0)} \,. \tag{12}$$

Recalling that in the present problem the eigenvalues of $\mathbf{W}$ are non-degenerate, the exponential term can be re-written as:

$$\mathbf{X(t)} = \mathbf{Y}\exp(-\mathbf{D}\,t)\mathbf{Y^{-1}}\,\mathbf{X(0)} \,, \tag{13}$$

where $\mathbf{Y}$ is the matrix of the eigenvectors of the matrix $\mathbf{W}$ and $\mathbf{Y}^{-1}$ its inverse. $\mathbf{D}$ is the diagonal matrix containing the eigenvalues of $\mathbf{W}$. There is a variety of ways at hand from the literature to compute the solution of equation (11) [10]. In the numerical calculation that follows, the matrix $\mathbf{W}$ is of order $8 \times N_1 \times N_2$ with values for N_1 and N_2 around 14 so that the matrix is of order $\sim 10^3$. This size is still manageable by the present procedure, as already shown in ref. [11]. We apply now the decomposition of the matrix $\mathbf{W}$ in a diagonal and off-diagonal contribution $\mathbf{W} = \mathbf{D} + \mathbf{U}$, where $\mathbf{D}$ is the diagonal part of $\mathbf{W}$ and $\mathbf{U}$ is the matrix with the remaining elements, then Eq. (11) becomes:

$$\mathbf{X'(t)} + \mathbf{DX(t)} \,= -\mathbf{UX(t)} \,. \tag{14}$$

Applying the decomposition method in close analogy to the case of the point kinetics model [8], we expand the transformed problem as a series and truncate it at order R:

$$\mathbf{X(t)} = \sum_{r=0}^{R} \mathbf{X_r(t)} \,, \tag{15}$$

where R is the number of recursive terms for the convergence of the series. The resulting recursive system is then

$$\frac{d}{dt}\mathbf{X_0(t)} + \mathbf{DX_0(t)} \,= 0 \,, \tag{16}$$

for the first term of the expansion of the solution (15) and

$$\frac{d}{dt}\mathbf{X_r(t)} + \mathbf{DX_r(t)} = -\mathbf{UX_{r-1}(t)}\ , \tag{17}$$

for any generic successive term for the expansion with $r = 1, \ldots, R$. The matrix decomposition of $\mathbf{W}$ allows one to work with matrices of huge order ($\sim 10^3$), since the solution of the homogeneous problem (16) is known and the non-homogeneous one may be obtained by recursion (17). More specifically, the initial and boundary conditions are matched using the diagonalised problem, whereas the non-diagonal contributions are subject to homogeneous boundary conditions.

Once the solution for the recursive system is determined, the specific value for R may be evaluated using a genuine convergence criterion. Thus, without applying truncations we have found an exact solution for the neutron flux and the neutron precursor yields using the formulas (7), (8) and (9). In order to show the efficiency of the proposed algorithm and evaluate the solution, in the following we discuss how to control the convergence and determine the truncation associated to a prescribed accuracy. To this end we reformulate the Cardinal Theorem of Interpolation for our purposes: "A square integrable function $\omega = \int_r \phi_i(x, y)\ dy \in L^2$ associated to eigenvalues λ_i and $i = 1, \ldots, N_{max}$ which is limited by $(m\Sigma_{Tg})^{-1}$ has an exact solution for a finite expansion". More specifically, knowing that the behaviour of the fast and thermal neutron fluxes are dominated by the values of the total cross sections (Σ_{Tg}) for each group, we can infer that between two successive neutron interactions, that is a path length of the order of the neutron mean free path ($\lambda_g = \Sigma_{Tg}^{-1}$), the neutron flux is unchanged. In other words the quantity $(m\Sigma_{Tg})^{-1}$ defines a sampling density in the spirit of Whittaker, Nyquist, Kotelnikov and Shannon [9]. Convergence is then given if an integer multiple of the neutron mean free path is determined such that beyond this value, the neutron flux value undergoes only small changes $< \epsilon$. The choice of m in turn is related to the number of terms N_{max} in the series for the region of interest, which depends on the precision of the solution. On the other hand, one may make use of Parseval's theorem to estimate the error bound of the solution. In the next section, we illustrate this procedure, attaining results by this procedure with an error of $< 1\%$ where only two terms in the series are sufficient, or in other words where the numerical solution may be obtained by a manageable formula. In the further we refer to the numerical implementation of the solution as GITTDM.

3. NUMERICAL RESULTS

In this section the solution of the previous section is used to reproduce the numerical results of ref. [12]. The transient considered in this reference was initiated by perturbing a steady-state situation. We also assume the delayed neutron precursor yields to be at their steady-state values. These initial conditions are generally obtained from calculations of time independent diffusion theory. For our considerations we used the initial condition of ref. [13]. We adopt two-energy groups where the neutron precursors appear in the thermal section of the spectrum only. The reactor is approximated as a homogeneous composition (see ref. [12]) with square dimension 200 cm $\times$ 200 cm and on the boundaries homogeneous Dirichlet conditions are introduced. The perturbation consists of a uniform step decrease in the absorption cross section of the second group by the amount $\Delta\Sigma_{a2} = -0.396 \times 10^{-4}$ cm^{-1}. The nuclear parameter values are given in Table I.

Table I: Nuclear data.

Material properties	Energy group (g)	
	1	2
D_g [cm]	1.35	1.08
Σ_{ag} [cm^{-1}]	0.001382	0.00569
ν	2.41	2.41
Σ_{fg} [cm^{-1}]	0.000242	0.00428
$\Sigma_{gg'}$ [cm^{-1}]	0.0023	0
$\lambda = 0.08$ [s^{-1}] $\beta = 0.0064$		
$k_{eff} = 1.000008$		

In Table II, the results are compared with the method GRK-4a proposed by Aboanber [12]. We show and compare the values for the thermal neutron flux at the centre of the reactor for several times. In order to produce numerical values that maintain the solution below an error level of 1%, two terms in the solution series are needed, together with five recursions (defined in Eq. (17)). As expected from our convergence analysis, a few terms in the eigenfunction expansion and an acceptable low number of recursions gives a good agreement with the results presented in ref. [12].

Table II: Comparison of the thermal neutron flux in the centre of the reactor for different times.

Time [s]	GITTDM [cm^{-2}s^{-1}]	GRK-4A [cm^{-2}s^{-1}]
0	0.380	0.382
0.08	0.612	0.613
0.16	0.817	0.818
0.24	0.996	0.996
0.32	1.155	1.155
0.4	1.304	1.304

4. CONCLUSIONS

In the present work we derived an exact solution for the kinetic neutron diffusion equation with delayed neutron precursor yields in terms of a well defined series. For a precision of the order of a percent only a few terms are required to reproduce numerically the exact solution of the problem in form of a relatively compact formula. Existence and uniqueness is guaranteed by the Cauchy-Kowalewsky theorem, further convergence of the solution is under control by a new interpretation of the Cardinal Theorem of Interpolation, where the macroscopic cross section plays the role of a sampling density and the reconstruction of the solution follows the common procedure in signal processing as introduced in independent works by Whittaker, Nyquist, Kotelnikov and Shannon (see ref. [14] and references therein).

The only task to be executed for applications is to determine numerically the GITT eigenvalues

and substitute the physical parameters and boundary conditions into the solutions which may be calculated directly. In order to get a comparable precision with numerical or stochastic procedures, more computational time is needed, because a numerical algorithm for each energy group and region has to be executed. This is a clear advantage, especially by virtue of the stiffness character of the problem that has its origin in considerable differences of physical time scales between the prompt and delayed neutrons (three orders of magnitude). With the present approach, no difficulties appear, such as instability, a common effect in numerical approaches for that type of problems. Furthermore, any analysis that focuses on the influences of modifications in geometry and material composition on the solution may be derived in a direct analytical fashion.

It is noteworthy, that the method developed is not restricted to the presented Cartesian geometry but can be extended to other geometries. Also the consideration of one homogeneous material composition of the domain does not restrict the generality of the procedure; the extension to a stepwise-constant heterogeneous system may be implemented following the reasoning of ref. [15]. Moreover, a substantial increase in the number of energy-groups and in the number of precursor families does not compromise the procedure, since no eigenvalue problem has to be solved, as a direct consequence of the decomposition of diagonal and off-diagonal contributions to the equation, that otherwise would restrict the order of the matrix system to be solved.

From the previous discussion, we envisage a natural and obvious extension of this sort of solution for the full three-dimensional space and time neutron kinetic diffusion equations by the spectral method approach. The characteristics of the integral transform technique permits an reduction of the order of the problem to successively lower dimensional cases, because of the invariance of the form of the solution regardless to the topology of the problem. In a future work we shall focus on the aforementioned extensions.

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