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Analytical representation of the solution of the space kinetic diffusion equation in a one-dimensional and homogeneous domain

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ABSTRACT

In this work we solve the space kinetic diffusion equation in a one-dimensional geometry considering a homogeneous domain, for two energy groups and six groups of delayed neutron precursors. The proposed methodology makes use of a Taylor expansion in the space variable of the scalar neutron flux (fast and thermal) and the concentration of delayed neutron precursors, allocating the time dependence to the coefficients. Upon truncating the Taylor series at quadratic order, one obtains a set of recursive systems of ordinary differential equations, where a modified decomposition method is applied. The coefficient matrix is split into two, one constant diagonal matrix and the second one with the remaining time dependent and off-diagonal terms. Moreover, the equation system is reorganized such that the terms containing the latter matrix are treated as source terms. Note, that the homogeneous equation system has a well known solution, since the matrix is diagonal and constant. This solution plays the role of the recursion initialization of the decomposition method. The recursion scheme is set up in a fashion where the solutions of the previous recursion steps determine the source terms of the subsequent steps. A second feature of the method is the choice of the initial and boundary conditions, which are satisfied by the recursion initialization, while from the first recursion step onward the initial and boundary conditions are homogeneous. The recursion depth is then governed by a prescribed accuracy for the solution.

Keywords: neutron diffusion equation, Taylor series, modified Adomian Decomposition method.

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1. INTRODUCTION

Our starting point is the neutron space kinetics equation considering the fast and thermal groups and with six delayed neutron precursor groups. The typical time scales present in this set of eight equations vary over six orders in magnitude, which characterizes the problem as stiff.

In numerical approaches for solving the equation system this property imposes on the one hand restrictions on the time step size and on the other hand sets limits for the maximum time interval that may be simulated by the solution. Hence, in the present work we propose an analytical procedure that eliminates stiffness and is less susceptible to limitations in the maximum feasible time interval. As a consequence, one gains a fast and stable convergence with an acceptable small computational effort and free of the afore mentioned stiffness.

In reference (CEOLIN et al., 2011) an analytical solution of the multi group neutron diffusion kinetic equation in a multilayered slab with one neutron precursor group was discussed. There the solution was obtained by a modified Adomian decomposition method, where the heterogeneous problem was cast into a set of recursive problems with constant parameters. The authors of reference (PETERSEN et al., 2011) address an analytical solution of the multi group neutron kinetics diffusion equation in a homogeneous parallelepiped, considering two energy groups and six groups of delayed neutron precursors, by applying the GITT (Generalized Integral Transform Technique). Reference (CEOLIN et al., 2015a) presents the multi-region bi-dimensional diffusion kinetics model with analytical expressions through the Taylor series, where the coefficients are found using the differential equation and the boundary and interface conditions. Using the same method, the authors also solved the one-dimensional (CEOLIN, 2014) and the two-dimensional stationary problem (CEOLIN at al., 2015b). The basic idea of the method consists in expanding the scalar neutron flux and concentration of delayed neutron precursors in a double Taylor series in the spatial and temporal variable, substitution of these expansions in the space kinetic equation and construction of a linear algebraic system that allows to calculate the coefficients of the expansion in series, by the application of the boundary conditions and continuity of flux and neutron current in the interfaces of the mesh. Further, the initial condition was determined using the same methodology but for the stationary problem (see reference (CEOLIN et al., 2013)). In the same context, (SCHRAMM, 2016) solved the two-dimensional space

kinetic equation using a polynomial approximation in a homogeneous rectangular domain, with non-homogeneous boundary conditions. Note, that the studies cited above use analytical continuation, that is, the successive integration in time to determine the solution.

In this work we determine a new solution free of stiffness and in analytical representation in one-dimensional geometry and a homogeneous domain. In summary, the methodology consists of expanding the scalar neutron flux and the concentration of delayed neutron precursors in Taylor series in the spatial variable (applying the methodology discussed in (CEOLIN, 2014), where the temporal dependence is incorporated in the coefficients of that series, that allows to decompose the original problem into a recursive system of time-dependent ordinary differential equations. We avert the stiffness character using the idea of (SILVA et al., 2014) (applied in the solution of the problem of neutron point kinetics) and thus obtaining the solution of the problem. The idea consists in splitting the coefficient matrix into two, one constant diagonal matrix and the second one with the remaining time dependent and off-diagonal terms. Moreover, the equation system is reorganized such that the terms containing the second matrix are assigned as source terms. The homogeneous equation system has a well known solution, since the matrix is diagonal and constant, and plays the role of the recursion initialization of the decomposition method (ADOMIAN, 1988; ADOMIAN and RACH, 1996; ADOMIAN, 1994; PETERSEN, 2011; SILVA et al., 2014). The recursion scheme is set up in a fashion where the solutions of the previous recursion steps determine the source terms of all subsequent steps. A second feature of the method is the choice satisfying the initial and boundary conditions by the recursion initialization, so that from the first recursion step onward initial and boundary conditions are homogeneous. The fact that the time evolution in the solution is calculated recursively for in principle all times does not impose any restrictions such as convergence limitations that are typically present in progressive time step approaches, used by the methods cited above and elsewhere.

2. MODEL AND METHODOLOGY

The methodology, presented in this section, aims to determine the solution of the neutron space kinetic equation (1) with two groups of energy, six groups of delayed neutron precursors, in one-dimensional

geometry and homogeneous domain. To this end a recursive scheme is elaborated, that avoids the otherwise inexorable presence of stiffness in the algorithm.

$$\begin{aligned}\frac{1}{v_1}\frac{\partial\Phi_1(x,t)}{\partial t} &= D_1\nabla^2\Phi_1(x,t)-\Sigma_{r1}\Phi_1(x,t)+(1-\beta)(\upsilon_1\Sigma_{f1}\Phi_1(x,t)+\upsilon_2\Sigma_{f2}\Phi_2(x,t))+\sum_{i=1}^{6}\lambda_i C_i(x,t),\\ \frac{1}{v_2}\frac{\partial\Phi_2(x,t)}{\partial t} &= D_2\nabla^2\Phi_2(x,t)-\Sigma_{a2}(t)\Phi_2(x,t)+\Sigma_{s12}\Phi_1(x,t),\\ \frac{\partial C_i(x,t)}{\partial t} &= \beta_i(\upsilon_1\Sigma_{f1}\Phi_1(x,t)+\upsilon_2\Sigma_{f2}\Phi_2(x,t))-\lambda_i C_i(x,t),\end{aligned} \tag{1}$$

where *i=1,...,6*. Here Φ_1 and Φ_2 denote the fast and the thermal neutron flux, C_i is the i-th delayed neutron precursor group concentration, v is the neutron velocity, *D* is the diffusion coefficient, Σ_a is the absorption cross section, Σ_s is the scattering cross section, Σ_f is the fission cross section, υ is the average number of neutrons emitted by fission, β is the delayed neutron fraction and the λ are the delayed neutron decay constants. The system of equation is subject to the initial conditions:

$$\begin{aligned}\Phi_1(x,0) &= \Phi_{1,0}(x),\\ \Phi_2(x,0) &= \Phi_{2,0}(x),\\ C_i(x,0) &= \frac{\beta_i}{\lambda_i}(\upsilon_1\Sigma_{f1}\Phi_{1,0}(x)+\upsilon_2\Sigma_{f2}\Phi_{2,0}(x)).\end{aligned} \tag{2}$$

One may think of a global domain segmented into a set of sufficiently small subdomains, where in each of those the solution is represented by a Taylor expansion in the spatial variable, where the expansion point is centered in the respective subdomain with size $2\Delta x$ and for convenience equal size intervals are understood.

$$\begin{aligned}\Phi_1(x,t) &= \sum_{n=0}^{\infty}A_n(t)(x-x_0)^n,\\ \Phi_2(x,t) &= \sum_{n=0}^{\infty}B_n(t)(x-x_0)^n,\\ C_i(x,t) &= \sum_{n=0}^{\infty}\mathcal{C}_{i,n}(t)(x-x_0)^n.\end{aligned} \tag{3}$$

Note, that time dependence is incorporated in the coefficients of the Taylor series. This implies that the original equation system may be dimensionally reduced to a recursive system of ordinary differential time-dependent equations, which are solved by a modified Adomian Decomposition Method. Applying the expansions (3) in the system of equations (1), results in:

$$\begin{aligned}
&\frac{1}{v_1}\frac{\partial}{\partial t}\sum_{n=0}^{\infty}A_n(t)(x-x_0)^n = D_1\sum_{n=0}^{\infty}(n+1)(n+2)A_{n+2}(t)(x-x_0)^n - \Sigma_{r1}\sum_{n=0}^{\infty}A_n(t)(x-x_0)^n \\
&+(1-\beta)(\upsilon_1\Sigma_{f1}\sum_{n=0}^{\infty}A_n(t)(x-x_0)^n + \upsilon_2\Sigma_{f2}\sum_{n=0}^{\infty}B_n(t)(x-x_0)^n) + \sum_{i=1}^{6}\lambda_i\sum_{n=0}^{\infty}\mathcal{C}_{i,n}(t)(x-x_0)^n, \\
&\frac{1}{v_2}\frac{\partial}{\partial t}\sum_{n=0}^{\infty}B_n(t)(x-x_0)^n = D_2\sum_{n=0}^{\infty}(n+1)(n+2)B_{n+2}(t)(x-x_0)^n - \Sigma_{a2}(t)\sum_{n=0}^{\infty}B_n(t)(x-x_0)^n \\
&+\Sigma_{s12}\sum_{n=0}^{\infty}A_n(t)(x-x_0)^n, \\
&\frac{\partial}{\partial t}\sum_{n=0}^{\infty}\mathcal{C}_{i,n}(t)(x-x_0)^n = \beta_i(\upsilon_1\Sigma_{f1}\sum_{n=0}^{\infty}A_n(t)(x-x_0)^n + \upsilon_2\Sigma_{f2}\sum_{n=0}^{\infty}B_n(t)(x-x_0)^n) - \lambda_i\sum_{n=0}^{\infty}\mathcal{C}_{i,n}(t)(x-x_0)^n,
\end{aligned} \tag{4}$$

Different powers *n* in *x* are linear independent so that terms with equal power have to vanish individually, which leads to the afore mentioned system of ordinary differential equations in the time variable.

$$\begin{aligned}
&\frac{\partial}{\partial t}A_n(t) + A_n(t)(v_1\Sigma_{r1} - (1-\beta)v_1\upsilon_1\Sigma_{f1}) + B_n(t)(-(1-\beta)v_1\upsilon_2\Sigma_{f2}) + \mathcal{C}_{i,n}(t)(-v_1\sum_{i=1}^{6}\lambda_i) = \\
&\qquad (n+1)(n+2)A_{n+2}(t)(D_1v_1), \\
&\frac{\partial}{\partial t}B_n(t) + A_n(t)(-v_2\Sigma_{s12}) + B_n(t)(v_2\Sigma_{a2}(t)) = (n+1)(n+2)B_{n+2}(t)(v_2D_2), \\
&\frac{\partial}{\partial t}\mathcal{C}_{i,n}(t) + A_n(t)(-\beta_i\upsilon_1\Sigma_{f1}) + B_n(t)(-\beta_i\upsilon_2\Sigma_{f2}) + \mathcal{C}_{i,n}(t)(\lambda_i) = 0.
\end{aligned} \tag{5}$$

For convenience one may represent this equation system in a matrix form,

$$\frac{d\mathbf{X}_n(t)}{dt} + \mathbf{W}(t)\mathbf{X}_n(t) = \mathbf{S}_n(t) \tag{6}$$

where $\mathbf{X}_n(t) = [A_n(t),\ B_n(t),\ \mathcal{C}_{i,n}(t)]^T$ $(i=1,...,6)$, $\mathbf{S}_n(t) = [(n+1)(n+2)A_{n+2}(t)(D_1v_1),$ $(n+1)(n+2)B_{n+2}(t)(D_2v_2), 0,0,0,0,0,0]^T$, and $\mathbf{W}(t)$ are the coefficients matrix of the system equations (5). Note that the coefficients $A_{n+2}(t)$ and $B_{n+2}(t)$ arising from the diffusive term of the fast and thermal flux equations were placed as source term.

The initialization together with the subsequent two equations of the ODE system are given in equation (7) and we evidently have to truncate the system in order to render this problem tractable from the computational point of view. Due to the Taylor expansion up to the second order the system of three coupled equations is to be solved.

$$\begin{aligned} \mathbf{X}'_0(t) + \mathbf{W}(t)\mathbf{X}_0(t) &= \mathbf{S}_0(t), \\ \mathbf{X}'_1(t) + \mathbf{W}(t)\mathbf{X}_1(t) &= 0, \\ \mathbf{X}'_2(t) + \mathbf{W}(t)\mathbf{X}_2(t) &= 0. \end{aligned} \tag{7}$$

Here the source term $\mathbf{S}_0(t)$ is related to details of the fast and thermal neutron current density.

In order to solve this coupled equation system we make use of a decomposition method in the spirit of some works in the literature (ADOMIAN, 1988; ADOMIAN and RACH, 1996; ADOMIAN, 1994; PETERSEN, 2011; SILVA et al., 2014). Note, that the present problem is a linear equation system, whereas in references (ADOMIAN, 1988; ADOMIAN and RACH, 1996; ADOMIAN, 1994) the presented method there was designed for non-linear problems, so that for the present procedure there is no need for determining the functional polynomials, only the expansion technique is employed in order to determine the expansion coefficients.

$$\begin{aligned} A_n(t) &= \sum_{j=0}^{J} A_{n,j}(t), \\ B_n(t) &= \sum_{j=0}^{J} B_{n,j}(t), \\ \mathcal{C}_{i,n}(t) &= \sum_{j=0}^{J} \mathcal{C}_{i,n,j}(t). \end{aligned} \tag{8}$$

Further, the matrix $\mathbf{W}(t)$ is split into a diagonal matrix $\mathbf{W}_0$ containing constant elements only, and a second matrix $\mathbf{W}_1(t)$ which contains the off-diagonal elements together with the time dependent terms. More specifically, in the present consideration the absorption cross section of the thermal neutron group is assumed to be time dependent $\Sigma_{a2}(t) = \Sigma_{a2,0} + \Sigma_{a2,1}(t)$. On the one hand this allows to decouple already in the recursion initialization equations with its associated time scales, which circumvents the otherwise appearing stiffness problem. As will be shown below the recursion system corrects then the solution until a prescribed precision is attained, i.e. the recursion depth is finite and stops at recursion step *J*.

Upon inserting the expansions (8) into the original differential equation system opens up for separating groups of terms, that setup the constitutive equations that determine the expansion coefficients $A_{n,j}(t)$, $B_{n,j}(t)$ and $\mathcal{C}_{i,n,j}(t)$. It is noteworthy that this splitting procedure is not unique, a variety of possibilities exist and the choice for the present scheme is based on the discussion of reference (Silva, 2014). Thus, the recursion prescription is given by the following equations, where for the recursion initialization the equation system is homogeneous and only for *j > 0* the system is non-homogeneous with the time dependent and off-diagonal terms as source terms and using the solution from the previous recursion step.

$$\begin{aligned} \mathbf{X}'_{0,j}(t) + \mathbf{W}_0\mathbf{X}_{0,j}(t) &= \mathbf{S}_{0,j-1}(t) - \mathbf{W}_1(t)\mathbf{X}_{0,j-1}(t), \\ \mathbf{X}'_{1,j}(t) + \mathbf{W}_0\mathbf{X}_{1,j}(t) &= -\mathbf{W}_1(t)\mathbf{X}_{1,j-1}(t), \\ \mathbf{X}'_{2,j}(t) + \mathbf{W}_0\mathbf{X}_{2,j}(t) &= -\mathbf{W}_1(t)\mathbf{X}_{2,j-1}(t). \end{aligned} \tag{9}$$

The solutions of equations (9) are known and given by equation (10).

$$\mathbf{X}_{n,j}(t) = \exp(-\mathbf{W}_0 t)\mathbf{X}_{n,j}(0) + \int_0^t \exp(-\mathbf{W}_0 t)\mathbf{Q}_{n,j}(t-\tau)d\tau. \tag{10}$$

Here $\mathbf{Q}_{n,j}$ represents the inhomogeneities of equations (9) and $\mathbf{X}_{n,j}(0)$ are determined from the initial conditions. The numerical results were generated using as initial condition the stationary solution from reference (CEOLIN, 2014b), which is absorbed in the recursion initialization $\mathbf{X}_{n,0}(0)$, whereas for *j > 0* the initial condition reads $\mathbf{X}_{n,j}(0) \equiv 0$.

By inspection one observes that the contribution from the time dependent nuclear parameters enters through the source term in the integral equation (10). For small times *t* the integral gives only small contributions whereas for large times the exponential term dominates the integrand, which also results in small contributions.

Only for times where the integrand is not small larger contributions to the solution appear. Moreover, the solution of the time evolution is corrected simultaneously for all times, so that the corrections in the time region where the integral has significant contributions determine the recursion depth according to a prescribed precision of the solution., a clear advantage in comparison to progressive methods such as the one in reference (TUMELERO, 2015).

The stiffness problem present in a variety of approaches does not appear in this method since the origin of the stiff character is manifest in the diagonal elements of the matrix $\mathbf{W}_0$. The corrections in the solution alter the components of each time scale separately since the matrix exponential in the integral is diagonal, so that the source term adds only terms to each contribution with its characteristic time scale.

3. NUMERICAL RESULTS

In order to demonstrate the feasibility of methodology, we apply the proposed method to neutron space kinetics in a homogeneous domain and one-dimensional geometry, with two energy groups and six groups of delayed neutron precursors. The domain is defined by a slab of length $l = 160$ cm with zero flux boundary conditions ($\Phi(0) = \Phi(l) = 0$). The increment used in the space variable was $\Delta x = 0.25$ cm. The nuclear parameters are presented in Table 1 and Table 2.

Table 1: Nuclear Parameters.

Parameter	**Fast group**	**Thermal group**
***D* [cm]**	1.0	0.5
***v* [cm/s]**	1.0×10^7	3.0×10^5
Σ_a **[cm^{-1}]**	0.02	0.08
Σ_{s12} **[cm^{-1}]**	0.01	0
$\upsilon\Sigma_f$ **[cm^{-1}]**	0.005	0.099

Table 2: Delayed neutron parameters.

i	β_i	λ_i **[s^{-1}]**
1	0.00025	0.0124
2	0.00164	0.0305
3	0.00147	0.111
4	0.00296	0.301
5	0.00086	1.14

6	0.00032	3.01

In Figures 1 and 2 are shown the spatial dependence of the fast and scalar flux, for three instances (*t= 1 s, 5 s, 10 s*). The decreasing time evolution classifies the regime as sub-critical.

Figure 1: ***Fast neutron flux***

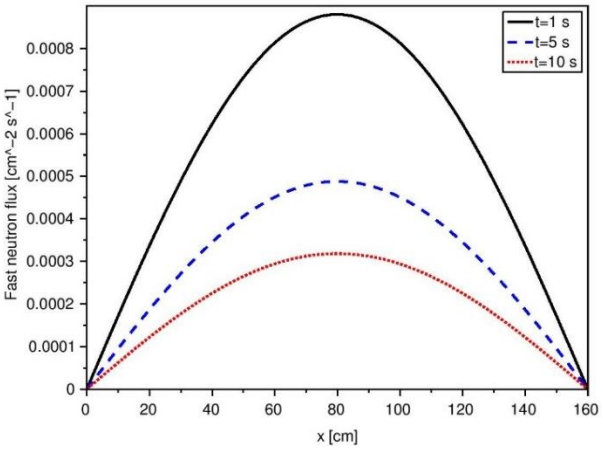
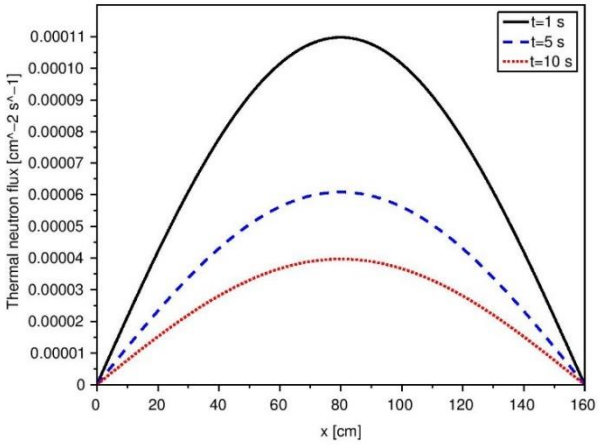


Figure 2: ***Thermal neutron flux***



To analyze the solution for fast and thermal flux, we vary the number of terms of the modified Decomposition Adomian Method. In the work developed by (CEOLIN, 2010), the same method was used to solve the temporal variable, but using the GITT method in the space variable with analytical continuation. In order to compare the number of terms needed to achieve the desired precision of the solution with the method mentioned in the literature, Table 3 presents the values of the neutron flux increasing the number *J* of terms of the expanded series in the time variable, at position *x = l/2* and for an instant *t = 1* s.

Table 3: Values of the fast and thermal fluxes increasing the terms of the modified Decomposition method.

J	Φ_1 **[cm^{-2}s^{-1}]**	Φ_2 **[cm^{-2}s^{-1}]**
2	0.00014454598	0.00001753745
10	0.00052324994	0.00006422107

20	0.00073721052	0.00009118650
30	0.00082348593	0.00010228426
40	0.00085788806	0.00010678391
50	0.00087148094	0.00010858685
100	0.00088012141	0.00010975359
150	0.00088019442	0.00010976394
200	0.00088019499	0.00010976394
300	0.00088019499	0.00010976394
400	0.00088019499	0.00010976394

From the results presented in Table 3, one observes that with 200 terms one attains the same accuracy as reference (CEOLIN, 2010). A comment is in order here, it seems that reference (CEOLIN, 2010) is more efficient due to the fact that there only 40 terms were needed to get results stable up to the eighth digit, however, both algorithms run with comparable CPU times. The principal difference in both approaches is that in reference (CEOLIN, 2010) time evolution was implemented making use of analytical continuation and hence needs the calculation of all time steps previous to the one of interest, whereas the present implementation allows to calculate directly the fluxes recursively for any desired time, i.e the present method does not employ a time step progressive scheme. The solutions for the thermal flux in Table 3 indicate that the precision of 8 digits was also achieved with 200 terms. The implemented method on this work shows its advantage over the one of reference (CEOLIN, 2010) if the knowledge of the fluxes for larger times are of interest. With increasing time the method in (CEOLIN, 2010) depends strongly on the chosen size of the time step Δt, which imposes limits on the convergence radius, whereas the method lined out in this work does not need any segmentation of the time axis.

4. CONCLUSION

In this work, we presented a solution for the space kinetics equation in analytical representation for one-dimensional and homogeneous domains. The method reduced the spatial part of the problem

using a segmented spatial domain, where the solution was expanded around the center of interval. This procedure reduced the original problem to a set of ODEs that determine the explicit time dependence of the expansion coefficients. Previous works in the literature made use of a progressive time-step scheme, which consequently has a relation between time step size and an upper time limit. The present implementation results in a recursive scheme that allows to determine the time dependence of the expansion coefficients where additionally the recursion formula for the polynomial coefficients in each recursion step with respect to time is split, such that coefficients of higher order are placed as source terms. From previous analysis not reported here the Taylor expansion in the spatial coordinate was restricted to the second order with associated domain segmentation size $2\Delta x$ in order to attain a prescribed precision. Comparing the new proposed method to reference (CEOLIN, 2010) shows that handling the time dependence with the expansion coefficients allows to solve for the time evolution using a decomposition method, where the recursion initialization is defined by the linear and diagonal (i.e. decoupled) matrix terms and the subsequent recursion steps contain the off-diagonal and time dependent nuclear parameters, which constitute the afore mentioned source terms. As a consequence stiffness manifest in the diagonal contributions remains uncoupled and enters in the solution of the recursion initialization, which consequently circumvents effects due to the stiff character of the equation system. Moreover, since the time evolution is determined in form of an analytical representation of the expansion coefficients, no time steps are necessary, in other words the solution is recursively improved for in principle any time. Evidently, error propagation that could impose limits on convergence is no issue in the present implementation. Also computational efforts are maintained reasonably small, which becomes especially apparent if solutions for larger time intervals ($>10^1$ s) shall be computed. As an extension in future works, we focus on heterogeneous domains as well as domains of higher dimensionality.

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