



The influence of half-range quadrature scheme on ADO method convergence

A influência do esquema de quadratura *half-range* na convergência do Método ADO

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Neste trabalho, é apresentada uma solução em ordenadas discretas para um problema de transporte de nêutrons em geometria cartesiana unidimensional. Buscando avaliar a eficiência do esquema de quadratura *half-range*, o método de Ordenadas Discretas Analítico (ADO) é utilizado para resolver duas classes de problemas em meios finitos e homogêneos (com espalhamento isotrópico e anisotrópico linear), para regime estacionário, sem fonte interna e com condições de contorno prescritas. Resultados numéricos para o fluxo escalar foram obtidos e comparações com outros trabalhos existentes na literatura foram feitas. A versatilidade quanto ao uso de quadraturas sempre foi vista como uma vantagem do método ADO que, além de fornecer resultados precisos a um baixo custo computacional, possui uma formulação mais simples, permitindo usar softwares de livre distribuição para as simulações. Na análise dos resultados, verificou-se que o uso da quadratura *half-range* foi capaz de acelerar a convergência, principalmente em problemas linearmente anisotrópicos.

Palavras-chave: equação de transporte unidimensional, quadratura *half-range*, anisotropia linear.

In this work, a discrete ordinates solution for a neutron transport problem in one-dimensional Cartesian geometry is presented. In order to evaluate the efficiency of the half-range quadrature scheme, the Analytical Discrete Ordinates method (ADO) is used to solve two classes of problems in finite and homogeneous media (with isotropic and linear anisotropic scattering), for steady-state regime, without inner source and prescribed boundary conditions. Numerical results for the scalar fluxes were obtained and comparisons with other works in the literature were made. The versatility of the use of quadratures has always been seen as an advantage of the ADO method which, besides providing accurate results at a low computational cost, has a simpler approach, allowing the use of free software distribution for the simulations. In the results analysis, it was verified that the use of the half-range quadrature was able to accelerate the convergence, mainly in linearly anisotropic problems.

Keywords: one-dimensional transport equation, half-range quadrature, linear anisotropy.

1. INTRODUCTION

In recent years, several methods have been proposed with the objective of finding solutions to the equations that model the phenomena of particle transport and radiation [1-6]. Among these, maybe the most important has been the Discrete Ordinates method (S_N method), which was the first deterministic method to be systematically applied to neutron transport problems [7, 8] with remarkable ability to deal with one-dimensional and multidimensional problems, in different levels of complexity.

Originally introduced by Wick (1943) [9] for solving neutron transport problems and later used by Chandrasekhar (1950) [10] in his radioactive transfer studies, the traditional S_N method basically transforms the integral-differential transport equation into a coupled system of differential equations, making a discrete representation of the directional variable and the scattering integral terms in the form of a quadrature. Thus, the obtained solutions are representations of the radiation intensities in a set of discrete directions comprised in the total solid angle range.

However, the implementation of this method presented some difficulties on the numerical point of view [11]. The limitation of the S_N quadrature as to the number of directions (in order to avoid physically unrealistic weighting factors), the difficulties when applied to more complex geometries [12], and the calculation of separation constants bound to the roots of complicated characteristic polynomials, make the use of S_N method susceptible to some restrictions or conditions.

In the years that followed, several approaches based on the S_N method were developed looking for computational gains and simpler treatment of more complex phenomena. Among these approaches, there is the Analytical Discrete Ordinates method (ADO), proposed by Barichello and Siewert (1999) [3].

The ADO method can be seen today as the most efficient approach for the treatment of one-dimensional transport and radiation problems. Among its advantages, the versatility on the use of quadratures, the separation constants obtained through reduced eigenvalue problems, and the construction of analytical solutions in terms of spatial variables can be highlighted. All these factors contribute to the ADO method's feature of providing accurate results at low computational cost.

Based on these considerations, especially concerning the flexibility of the ADO method on the use of quadratures, this work will explore the computational aspects of the half-range (or double-gauss) quadrature schemes and provide some benchmark results for one-dimensional transport problems in homogeneous media with isotropy and linear anisotropy effects.

For this, the results obtained by ADO_{2N} method (with half-range Gauss-Legendre quadrature) will be compared with those obtained through other analytical and numerical formulations using full-range quadrature, including the ADO method itself.

2. PROBLEM FORMULATION

According to Barichello (1992) [1], the neutron transport equation in one-dimensional Cartesian geometry, for a homogeneous medium with isotropic and linearly anisotropic scattering in steady-state regime is given by

$$\mu \frac{d}{dx} \Psi(x, \mu) + \sigma_t \Psi(x, \mu) = \frac{\sigma_{s0}}{2} \int_{-1}^1 \Psi(x, \mu') d\mu' + \frac{3}{2} \sigma_{s1} \mu \int_{-1}^1 \mu' \Psi(x, \mu') d\mu' \quad (1)$$

where x [cm] and μ correspond to the spatial and directional variables wherein the angular fluxes $\Psi(x, \mu)$ [n/cm²·s] are calculated, σ_t [cm⁻¹], σ_{s0} [cm⁻¹] and σ_{s1} [cm⁻¹] are, respectively, the total, isotropic and linearly anisotropic macroscopic cross section. Here, in particular, only problems without inner sources will be considered, and the fluxes will be caused by prescribed boundary conditions, Figure 1. So, particular solutions are not necessary.

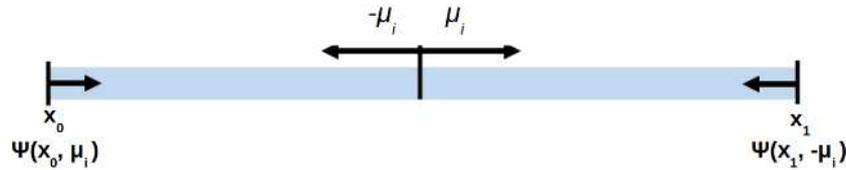


Figure 1. Domain representation of the problems.

For application of the ADO method, the integral terms must be modified. So, according to Barichello and Siewert (1999) [3]:

$$\int_{-1}^1 \Psi(x, \mu') d\mu' = \int_0^1 [\Psi(x, \mu') + \Psi(x, -\mu')] d\mu', \quad (2)$$

$$\int_{-1}^1 \mu' \Psi(x, \mu') d\mu' = \int_0^1 \mu' [\Psi(x, \mu') - \Psi(x, -\mu')] d\mu'. \quad (3)$$

After that, these integral terms are approximated by a numerical quadrature [10], such as

$$\int_0^1 [\Psi(x, \mu') + \Psi(x, -\mu')] d\mu' = \sum_{k=1}^N w_k [\Psi(x, \mu_k) + \Psi(x, -\mu_k)], \quad (4)$$

$$\int_0^1 \mu' [\Psi(x, \mu') - \Psi(x, -\mu')] d\mu' = \sum_{k=1}^N \mu_k w_k [\Psi(x, \mu_k) - \Psi(x, -\mu_k)], \quad (5)$$

where w_k are the weights associated with points μ_k when the discretization of the integral term is made by a quadrature scheme defined in $[0, 1]$.

According to Wick (1943) [9], the weights and points should be chosen based on Gaussian quadrature formula, so that the discretization of the integral terms will be exact for any polynomial written in powers of μ with degree less or equal than $2N-1$.

In this work, the half-range scheme associated with Gauss-Legendre quadrature will be explored, due to their relevant advantages shown in several works [13-16]. In order to adapt the Gauss Legendre quadrature to Eqs. (4)-(5), a mapping of the discrete directions (and associated weights) must be made in order to convert the interval $[-1,1]$ into $[0,1]$. For this, the following variable changes are performed

$$2\mu_k = y_k + 1, \quad (6)$$

$$2w_k = v_k, \quad (7)$$

where y_k and v_k represent, respectively, points and weights of the full-range Gauss Legendre quadrature ($[-1,1]$), and points μ_k and weights w_k are their representatives in the half-range quadrature scheme ($[0,1]$). In this step, the ADO method associated with half-range quadrature, to distinguish it from other traditional methods, will be called ADO_{2N}.

After that, it is possible to write a discrete ordinates version of Eq. (1), such that

$$\begin{aligned} \mu_i \frac{d}{dx} \Psi(x, \mu_i) + \sigma_i \Psi(x, \mu_i) = \frac{\sigma_{s0}}{2} \sum_{k=1}^N w_k [\Psi(x, \mu_k) + \Psi(x, -\mu_k)] + \\ \frac{3}{2} \sigma_{s1} \mu_i \sum_{k=1}^N \mu_k w_k [\Psi(x, \mu_k) - \Psi(x, -\mu_k)] \end{aligned} \quad (8)$$

and

$$\begin{aligned} -\mu_i \frac{d}{dx} \Psi(x, -\mu_i) + \sigma_i \Psi(x, -\mu_i) = \frac{\sigma_{s0}}{2} \sum_{k=1}^N w_k [\Psi(x, \mu_k) + \Psi(x, -\mu_k)] - \\ \frac{3}{2} \sigma_{s1} \mu_i \sum_{k=1}^N \mu_k w_k [\Psi(x, \mu_k) - \Psi(x, -\mu_k)], \end{aligned} \quad (9)$$

for $i=1, \dots, N$, being N the number of discrete directions of Gauss-Legendre quadrature set, with μ_i representing the positive directions and $-\mu_i$ the negative ones.

3. ADO METHOD SOLUTION

Starting from the one-dimensional transport equation, Eq. (1), a system of differential equations is created, Eqs. (8)-(9), in which the ADO method [3] is easily applicable.

Thus, seeking homogeneous solutions in terms of eigenvalues and eigenfunctions, it is proposed that the angular fluxes be decomposed in the form

$$\Psi(x, \pm\mu_i) = \Phi(\nu, \pm\mu_i) e^{-x/\nu}, \quad (10)$$

for $i=1, \dots, N$, where the separation constants ν are associated with elementary solutions $\Phi(\nu, \pm\mu_i)$.

Now, substituting Eq. (10) into Eqs. (8)-(9), a coupled algebraic system is obtained

$$\begin{aligned} -\frac{\mu_i}{\nu} \Phi(\nu, \mu_i) + \sigma_i \Phi(\nu, \mu_i) = \frac{\sigma_{s0}}{2} \sum_{k=1}^N w_k [\Phi(\nu, \mu_k) + \Phi(\nu, -\mu_k)] + \\ \frac{3}{2} \sigma_{s1} \mu_i \sum_{k=1}^N \mu_k w_k [\Phi(\nu, \mu_k) - \Phi(\nu, -\mu_k)] \end{aligned} \quad (11)$$

and

$$\frac{\mu_i}{\nu} \Phi(\nu, -\mu_i) + \sigma_i \Phi(\nu, -\mu_i) = \frac{\sigma_{s0}}{2} \sum_{k=1}^N w_k [\Phi(\nu, \mu_k) + \Phi(\nu, -\mu_k)] - \frac{3}{2} \sigma_{s1} \mu_i \sum_{k=1}^N \mu_k w_k [\Phi(\nu, \mu_k) - \Phi(\nu, -\mu_k)], \quad (12)$$

for $i=1, \dots, N$.

Then, two auxiliary equations are defined

$$U(\nu, \mu_i) = \Phi(\nu, \mu_i) + \Phi(\nu, -\mu_i), \quad (13)$$

$$V(\nu, \mu_i) = \Phi(\nu, \mu_i) - \Phi(\nu, -\mu_i) \quad (14)$$

such that, if Eqs. (11)-(12) are added, the relation

$$V(\nu, \mu_i) = \frac{\nu}{\mu_i} \left[\sigma_i U(\nu, \mu_i) - \sigma_{s0} \sum_{k=1}^N w_k U(\nu, \mu_k) \right] \quad (15)$$

is obtained. On the other hand, subtracting Eq. (12) from Eq. (11), another relation between $U(\nu, \mu_i)$ and $V(\nu, \mu_i)$ can be written, and it is given by

$$-\frac{\mu_i}{\nu} U(\nu, \mu_i) + \sigma_i V(\nu, \mu_i) = 3\sigma_{s1} \mu_i \sum_{k=1}^N w_k \mu_k V(\nu, \mu_k). \quad (16)$$

Once the Eqs. (15)-(16) are obtained, algebraic manipulations can be performed in order to build an eigenvalues problem in terms of $U(\nu, \mu_i)$. This way

$$\frac{1}{\nu^2} U(\nu, \mu_i) = \frac{\sigma_i^2}{\mu_i^2} U(\nu, \mu_i) - \sum_{k=1}^N w_k U(\nu, \mu_k) \left[\frac{\sigma_i \sigma_{s0}}{\mu_i^2} + 3\sigma_i \sigma_{s1} - 3\sigma_{s0} \sigma_{s1} \left(\sum_{j=1}^N w_j \right) \right], \quad (17)$$

for $i=1, \dots, N$, which matrix representation can be made as

$$[D - A]\vec{U} = \lambda \vec{U}, \quad (18)$$

where \vec{U} is a vector with components $U(\nu, \mu_i)$,

$$\lambda = \frac{1}{\nu^2}, \quad (19)$$

and the matrices $N \times N$ associated with the system are such that

$$D = \text{diag} \left[\left(\frac{\sigma_1^2}{\mu_1^2} \right), \left(\frac{\sigma_2^2}{\mu_2^2} \right), \dots, \left(\frac{\sigma_N^2}{\mu_N^2} \right) \right] \quad (20)$$

and

$$A(i, k) = w_k \left[\frac{\sigma_i \sigma_{s0}}{\mu_i^2} + 3\sigma_i \sigma_{s1} - 3\sigma_{s0} \sigma_{s1} \left(\sum_{j=1}^N w_j \right) \right], \quad (21)$$

for $i, k=1, \dots, N$.

With the eigenvalues problem solved, λ_j for $j=1, \dots, N$ are determined and used to compute ν_j on Eq. (19). Besides that, $U(\nu_j, \mu_i)$ is used on Eq. (15) to obtain $V(\nu_j, \mu_i)$. Thus, by Eqs. (13)-(14), the elementary solutions can be written as

$$\Phi(v_j, \mu_i) = \frac{1}{2} [U(v_j, \mu_i) + V(v_j, \mu_i)], \tag{22}$$

$$\Phi(v_j, -\mu_i) = \frac{1}{2} [U(v_j, \mu_i) - V(v_j, \mu_i)], \tag{23}$$

for $i, j = 1, \dots, N$.

In this case, since the separation constants occur in pairs, $\{\pm v_j\}$, with real values, a symmetry is imposed in order to build a linearly independent basis of elementary solutions. For that

$$\Phi(v_j, \mu_i) = \Phi(-v_j, -\mu_i), \tag{24}$$

$$\Phi(v_j, -\mu_i) = \Phi(-v_j, \mu_i), \tag{25}$$

for $i, j = 1, \dots, N$.

Thus, the homogeneous solutions for Eqs. (8)-(9) can be written, explicitly, as

$$\Psi(x, \mu_i) = \sum_{j=1}^N A_j \Phi(v_j, \mu_i) e^{-(x-x_0)/v_j} + A_{j+N} \Phi(-v_j, \mu_i) e^{-(x_1-x)/v_j}, \tag{26}$$

$$\Psi(x, -\mu_i) = \sum_{j=1}^N A_j \Phi(v_j, -\mu_i) e^{-(x-x_0)/v_j} + A_{j+N} \Phi(-v_j, -\mu_i) e^{-(x_1-x)/v_j}, \tag{27}$$

for $i = 1, \dots, N$.

Note that the coefficients A_j on Eqs. (26)-(27) will be determined from the boundary conditions. As a particular case, only prescribed boundary conditions will be used here. So

$$\Psi(x_0, \mu_i) = F, \tag{28}$$

$$\Psi(x_1, -\mu_i) = G, \tag{29}$$

for $i = 1, \dots, N$ and F, G constant functions.

Once the solutions are established, including the values of all A_j coefficients, some quantities can be evaluated for comparison with the literature and analysis of the certain parameter effects. The focus of this work will be to explore the influence of quadratures on the scalar flux, according Lewis and Miller (1984) [17], is defined by

$$\phi(x) = 1/2 \int_{-1}^1 \Psi(x, \mu') d\mu', \tag{30}$$

which discrete ordinate version will be

$$\phi(x) = \frac{1}{2} \sum_{k=1}^N w_k [\Psi(x, \mu_k) + \Psi(x, -\mu_k)]. \tag{31}$$

4. NUMERICAL RESULTS AND COMPUTATIONAL ASPECTS

The problems chosen for discussion are those which physical properties are described on Table 1. Here, results obtained by different methods will be compared, as well as an analysis of used quadrature will be made.

Table 1-Physical parameters used in each problem.

Problem	Quantity of Interest	Characteristics	σ_t	σ_{s0}	σ_{s1}	F	G	$[x_0, x_1]$
1	Scalar Flux	Homogeneous Isotropic	1.0	0.97	0.0	2.0	2.0	$[0.0, 50.0]$
2	Scalar Flux	Homogeneous Anisotropic	1.0	0.99	0.8	1.0	0.0	$[0.0, 100.0]$

In Problem 1, characterized by considering the phenomenon in an isotropic homogeneous medium with incident angular fluxes at both domain ends, scalar flux profiles, Eq. (31), obtained by ADO_{2N} method was compared with the literature [18] for validation of code and method.

The values obtained by the ADO_{2N} method for Problem 1 (Table 2) demonstrate fast convergence of the results as the value of N increases, as well the coherence of the profiles in relation to parameters used in the simulations. In special, $N = 4$ is enough to get a convergence between five and six significant digits.

The validation can also be performed with Nunes and Barros (2009) [18], which solved this same test case by three different methods: Diamond Difference method (DD), Step and CN method. In all methods, besides using the discrete ordinates version of the transport equation with S_N quadrature on the interval $[-1, 1]$, the spatial variable is treated numerically [17].

Table 2: Problem 1 - Convergence analysis and results validation for scalar flux profiles computed by ADO_{2N} method and the literature [18].

x	ADO _{2N}				DD	Step	CN
	N=2	N=4	N=6	N=8	N=8	N=8	N=8
0.0	1.704731	1.704731	1.704731	1.704731	1.704731	1.703435	1.704683
0.5	0.366976	0.366806	0.366807	0.366807	-	-	-
10.0	0.083274	0.083341	0.083341	0.083341	-	-	-
15.0	0.018941	0.018983	0.018983	0.018983	-	-	-
20.0	0.004507	0.004523	0.004523	0.004523	-	-	-
25.0	0.001945	0.001954	0.001954	0.001954	0.001956	0.002012	0.001958
30.0	0.004507	0.004523	0.004523	0.004523	-	-	-
35.0	0.018941	0.018983	0.018983	0.018983	-	-	-
40.0	0.083274	0.083341	0.083341	0.083341	-	-	-
45.0	0.366976	0.366806	0.366807	0.366807	-	-	-
50.0	1.704731	1.704731	1.704731	1.704731	1.704731	1.703435	1.704683

In terms of agreement, as can be seen on Table 2, the results obtained here by the ADO_{2N} method are very similar to those presented by Nunes and Barros (2009) [18], being particularly closer to DD method. Despite the convergence being faster in isotropic problems, the use of the ADO method becomes computationally cheaper, since it does not need to use higher quadratures orders to obtain good results and it does not involve iterative processes or interpolation schemes.

Problem 2 deals with transport phenomenon in a homogeneous medium liable to influence of linear anisotropic scattering, and the right border of the domain is isolated ($G=0.0$). For this problem again it was chosen to calculate the scalar flux and comparisons with Barichello (1992) [1], Barros and Larsen (1990) [4] and Barbosa (2018) [19] were made.

Table 3: Problem 2 - Convergence analysis and results validation for scalar flux profiles computed by ADO_{2N} method and the literature [1, 4].

x	ADO _{2N}			LTS _N	SFG _N
	N = 4	N = 6	N = 8	N = 8	N = 8
0.0	0.82299	0.82299	0.82299	0.82284	0.82284
10.0	0.36023	0.36023	0.36023	-	-
20.0	0.16653	0.16654	0.16654	-	-
30.0	0.76992x10 ⁻¹	0.76993x10 ⁻¹	0.76993x10 ⁻¹	-	-
40.0	0.35593x10 ⁻¹	0.35593x10 ⁻¹	0.35593x10 ⁻¹	-	-
50.0	0.16452x10 ⁻¹	0.16452x10 ⁻¹	0.16452x10 ⁻¹	0.16471x10 ⁻¹	0.16470x10 ⁻¹
60.0	0.75988x10 ⁻²	0.75989x10 ⁻²	0.75989x10 ⁻²	-	-
70.0	0.34977x10 ⁻²	0.34977x10 ⁻²	0.34977x10 ⁻²	-	-
80.0	0.15838x10 ⁻²	0.15838x10 ⁻²	0.15838x10 ⁻²	-	-
90.0	0.66037x10 ⁻³	0.66037x10 ⁻³	0.66037x10 ⁻³	-	-
100.0	0.12221x10 ⁻³	0.12222x10 ⁻³	0.12222x10 ⁻³	0.12251x10 ⁻³	0.12250x10 ⁻³

The LTS_N formulation [1] is a semi-analytical method (as ADO_{2N} method) where, after the discrete ordinates approximation of Eq. (1), an algebraic system is generated by application of Laplace Transform on x variable. The SFG_N method [4] works like the numerical methods reported

on Problem 1, though Green's function is used on the iterative process. In particular, both methods use the full-range Gauss-Legendre quadrature to approximate the scattering integrals.

Considering the results on Table 3, despite all the good features of the ADO_{2N} method, such as the analyticity of the solutions, the independence of numerical schemes, or not having to deal with complex variables, a concordance no greater than three digits was obtained with LTS_N and SGF_N methods.

Table 4: Problem 2 - Convergence test of scalar flux profiles, comparing the ADO_N [19] and ADO_{2N} methods.

N	0 cm		50 cm		100 cm	
	ADO_N	This work ADO_{2N}	ADO_N	This work ADO_{2N}	ADO_N	This work ADO_{2N}
2	0.81725596	0.82305738	0.01699118	0.01643780	0.00012918	0.00012191
4	0.82225559	0.82299577	0.01653759	0.01645200	0.00012352	0.00012221
8	0.82283610	0.82299466	0.01647049	0.01645213	0.00012250	0.00012222
16	0.82295703	-	0.01645649	-	0.00012228	-
32	0.82298544	-	0.01645320	-	0.00012223	-
64	0.82299236	-	0.01645240	-	0.00012222	-
128	0.82299407	-	0.01645220	-	0.00012222	-
256	0.82299450	-	0.01645215	-	0.00012222	-
512	0.82299460	-	0.01645214	-	0.00012222	-

However, this same problem was recently studied by Barbosa (2018) [19], who used a version of the ADO method associated with full-range Gauss-Legendre quadrature (which will be referred here as ADO_N method), and also had their results compared with those obtained by LTS_N and SGF_N . There, using ADO_N for $N=8$, the same agreement with the literature in terms of significant digits was obtained and, only with $N=64$ it was able to reproduce the values obtained here by ADO_{2N} with $N=8$ (Table 4). Thus, it can be said that the results presented on Table 3 for ADO_{2N} with $N=8$ are convergent and reliable, confirming the convergence acceleration by half-range quadrature scheme.

It was already observed in other works [20, 21] that the inclusion of anisotropy effects in the phenomenon makes the convergence slower, indicating the importance to associate the half-range quadrature with ADO method in terms of computational time and processing.

5. CONCLUSIONS

In this work it was possible to verify the efficiency when the half-range quadrature scheme is associated with ADO method on the solution of transport problems in homogeneous media, mainly when anisotropy effects are considered. In particular, Problems 1 and 2, here described, had already been analyzed using the ADO method, but no study had been done in the sense of verifying the quadrature type influence on the results convergence yet.

In the scalar flux profiles obtained for Problem 1, the agreement between different numerical methods and ADO_{2N} method is clear, validating the methodology presented and the implemented code. Once it is a problem in isotropic medium, as already proven in previous studies, there are no major difficulties in terms of convergence, making it not necessary to use high order quadratures. In this sense, the contribution of ADO method here is to be a methodology of low computational cost, since: i) solutions of the homogeneous problem are analytical in terms of the spatial variable, avoiding the construction of computational meshes and the use of iterative schemes or interpolation processes; ii) the separation constants calculated by the eigenvalues problem in ADO_{2N} method present, when compared to other formulations in the available literature based on S_N method, a lower order.

On the other hand, on the results generated for Problem 2, the convergence acceleration by changing the quadrature from full-range Gauss-Legendre to half-range scheme is evident. In particular, it is shown the versatility of ADO method in the use of quadratures for the scattering

term integrals. The fact of using fewer terms on the quadrature implies the obtention of smaller systems, reducing processing time.

It is also important to emphasize that, for the cases here tested, the computational effort was relatively low, spending less than two seconds (in a 3.10 GHz Intel Core I7 processor with 8GB of RAM) to generate each profile. Moreover, the simplicity of the method allowed the use of free distribution software (Octave 4.2.1) for computational implementation.

In future works, the intention is to maintain the use of ADO method associated with half-range quadrature scheme in solving more general one-dimensional transport problems, with higher degrees of anisotropy, internal sources and determination of other important physical quantities.

6. ACKNOWLEDGMENTS

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