On the use of Analytical Techniques for Source Reconstruction Problems

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Abstract - *The Analytical Discrete Ordinates method for adjoint transport problems is applied in the solving process of an inverse problem of neutral particles source reconstruction in a physical medium with known properties and geometry.*

I. INTRODUCTION

Source estimation of nuclear particles is of utmost relevance in the effort against nuclear proliferation. A tool that might aid in the solution of such problems is the *Analytical Discrete Ordinates* (ADO) method, a version of the S_n method characterized for obtaining explicit solutions, with respect to the spatial variable, for the one-dimensional transport equation and its adjoint form [1, 2]. Recent studies also point out [3] that the ADO method along with nodal techniques, when applied in bi-dimensional problems, are able to reproduce results as accurate as other techniques from coarser meshes, which might provide a speed up in computational time.

In this work, the ADO adjoint solution is applied to solve an inverse problem of neutral particle source reconstruction in a medium with known physical properties and geometry, which results in a finite dimensional linear inverse problem [4].

II. MATHEMATICAL FORMULATION

Given an isotropic source of neutral particles S, the distribution of particles in one-dimensional slab geometry is obtained as the solution of the transport problem

$$\mathcal{L}\psi = S, \tag{1}$$

with the transport operator $\mathcal{L}$ written as [5]

$$\mathcal{L}\psi(z,\mu) = \mu\frac{\partial}{\partial z}\psi(z,\mu) + \sigma\psi(z,\mu) - \frac{c}{2}\sum_{l=0}^{L}\beta_l P_l(\mu)\int_{-1}^{1} P_l(\mu')\psi(z,\mu')d\mu' \tag{2}$$

where ψ is the angular flux of particles, in this work assumed to be symmetrical with respect to the azimuthal variable; $\mu \in [-1,1]$ is the cosine of the polar angle measured from the positive z-axis, with $z \in (0, z_0)$. Moreover, the total macroscopic cross-section is represented by σ, c is the mean number of neutral particles emerging from collisions, and β_l's are the coefficients of the expansion of the scattering in terms of Legendre's polynomials P_l's. Additionally, boundary conditions on the inward directions are prescribed as

$$\psi(0,\mu) = g_1(\mu) + \alpha_1\psi(z,-\mu), \tag{3a}$$

$$\psi(z_0,-\mu) = g_2(\mu) + \alpha_2\psi(z_0,\mu), \tag{3b}$$

for $\mu \in [0,1]$, with known incoming fluxes at the boundaries g_1 and g_2, and $\alpha_1, \alpha_2 \in [0,1]$, the reflection coefficients.

If σ_d is the absorption macroscopic cross-section of a neutral particles detector located within $(0, z_0)$, then [5]

$$r = \langle\psi, \sigma_d\rangle \equiv \int_0^{z_0}\int_{-1}^{1}\sigma_d(z,\mu)\psi(z,\mu)d\mu dz \tag{4}$$

is a measure of the absorption rate of neutral particles by the detector. In this formulation, σ_d is defined as a positive constant in a given contiguous region of $(0, z_0)$ and zero outside the region. Thus, r measures the absorption rate of neutral particles within the detector's region migrating from all possible directions.

Closely related to the transport operator $\mathcal{L}$, the adjoint transport operator $\mathcal{L}^\dagger$ is defined by [5]

$$\mathcal{L}^\dagger\psi^\dagger(z,\mu) = -\mu\frac{\partial}{\partial z}\psi^\dagger(z,\mu) + \sigma\psi^\dagger(z,\mu) - \frac{c}{2}\sum_{l=0}^{L}\beta_l P_l(\mu)\int_{-1}^{1} P_l(\mu')\psi^\dagger(z,\mu')d\mu' \tag{5}$$

where all physical parameters are the same as the ones in the transport operator $\mathcal{L}$. The rate of absorption of neutral particles defined in Equation (4) might be alternatively computed as [5]

$$r = \left\langle\psi^\dagger, S\right\rangle - P\left(g_1, g_2, \psi^\dagger\right) \tag{6}$$

by means of solving the adjoint transport problem

$$\mathcal{L}^\dagger\psi^\dagger = \sigma_d \tag{7}$$

subjected to boundary conditions prescribed by

$$\psi^\dagger(0,-\mu) = \alpha_1\psi^\dagger(z,\mu), \tag{8a}$$

$$\psi^\dagger(z_0,\mu) = \alpha_2\psi^\dagger(z_0,-\mu), \tag{8b}$$

for $\mu \in [0,1]$. The term $P\left(g_1, g_2, \psi^\dagger\right)$ represents a contribution of particles migrating on both inward and outward directions at $z = 0$ and $z = z_0$ and is given by

$$P\left(g_1, g_2, \psi^\dagger\right) = -\int_0^1 \mu\left[g_1(\mu)\psi^\dagger(0,\mu) + g_2(\mu)\psi^\dagger(z_0,-\mu)\right]d\mu. \tag{9}$$

III. SOURCE RECONSTRUCTION STRATEGY

Following Hykes and Azmy [4], a set of D particle detectors are placed within the physical domain $[0, z_0]$; for each detector, the adjoint angular flux that solves $\mathcal{L}^\dagger\psi^\dagger = \sigma_{d,i}$ is known, with $\sigma_{d,i}$ the absorption macroscopic cross section of the i-th detector; the original source of neutral particles S might be accurately approximated by the projection of S onto a linear space with known basis function f_j, $j = 1, \ldots, B$, i.e., S might be approximated by

$$\hat{S}(z) = \sum_{j=1}^{B} \alpha_j f_j(z), \tag{10}$$

with constants α_j yet to be found, i.e., targets of our source reconstruction process. Under these assumptions, the rate of absorption of neutral particles within the i-th detector region might be computed by

$$\begin{aligned} r_i &= \left\langle \psi_i^\dagger, \hat{S} \right\rangle - P\left(g_1, g_2, \psi_i^\dagger\right) \\ &= \sum_{j=1}^{B} \alpha_j \left\langle \psi_i^\dagger, f_j \right\rangle - P\left(g_1, g_2, \psi_i^\dagger\right) \end{aligned} \tag{11}$$

for $i = 1, \ldots, D$. Upon defining $\boldsymbol{r} = [r_i] \in \mathbb{R}^D$, $\boldsymbol{p} = \left[P\left(g_1, g_2, \psi_i^\dagger\right)\right] \in \mathbb{R}^D$ and $\boldsymbol{A} = \left[\left\langle \psi_i^\dagger, f_j \right\rangle\right] \in \mathbb{R}^{D\times B}$, Equation (11) is rewritten in vector form as

$$\boldsymbol{r} = \boldsymbol{A}\boldsymbol{\alpha} - \boldsymbol{p} \tag{12}$$

with $\boldsymbol{\alpha} = \left[\alpha_j\right] \in \mathbb{R}^B$. It is remarked here that the explicit dependence of Equation (6) on the source of neutral particles S allows one to reevaluate the detectors' readings vector $\boldsymbol{r}$ without needing to recompute the adjoint angular flux $\psi_i^\dagger$. Furthermore, since this dependence is linear and given the approximation of S by $\hat{S}$, the readings $\boldsymbol{r}$ are linearly related to the weights α_j of Equation (10), which allows the derivation of a linear inverse problem.

If for each neutral particle detector a noisy measurement $r_{m,i}$ is made available, computed by numerical simulation or obtained through physical experimentation, the coefficients α_j in Equation (10) are to be estimated by the minimization of the objective function [4]

$$f(\boldsymbol{\alpha}) = \|\boldsymbol{r}' - \boldsymbol{A}\boldsymbol{\alpha}\|_2^2, \tag{13}$$

with $\boldsymbol{r}' = \boldsymbol{r}_m - \boldsymbol{p}$, $\boldsymbol{r}_m = [r_{m,i}] \in \mathbb{R}^D$.

In this work, only sectionally constant approximations are considered to the neutral particle source S, thus, given $[0, z_0] = \bigcup_{j=1}^{B}[z_{j-1}, z_j]$, a partition of the physical domain, a function basis is defined as [4]

$$f_j(z) = \begin{cases} 1, & \text{if } z \in [z_{j-1}, z_j], \\ 0, & \text{otherwise.} \end{cases} \tag{14}$$

Since the space generated by the basis functions in Equation (14) might be too poor for the true space of the particle source S, the well known ill-posedness of inverse problems might negatively affect the quality of the reconstruction. This problem is treated here by searching for Tikhonov regularized solutions of a minimization problem, i.e, looking for solutions that minimize the objective function [6]

$$f_\lambda(\boldsymbol{\alpha}) = \|\boldsymbol{r}' - \boldsymbol{A}\boldsymbol{\alpha}\|_2^2 + \lambda^2\|\boldsymbol{\alpha}\|_2^2, \tag{15}$$

where λ is the Tikhonov's regularization parameter, here chosen by the *Morozov discrepancy principle* [6].

IV. AN ANALYTICAL FORMULATION TO THE ADJOINT TRANSPORT EQUATION

The inversion strategy previously described requires the adjoint transport equation $\mathcal{L}^\dagger\psi^\dagger = S^\dagger$ to be solved for each detector. A fast, concise and accurate approach is the *Analytical Discrete Ordinates* (ADO) method, originally derived by Barichello and Siewert [1] for the transport equation and extended by Pazinatto et. al. [2] to the adjoint transport equation.

Since Equation (5) is linear, the solution $\psi^\dagger$ is written as the solution of the homogeneous equation $L^\dagger\psi_h^\dagger = 0$ plus any particular solution. For the sake of simplicity, all physical parameters are considered constant. If sectionally constant, the domain is partitioned in regions of constant parameters, and continuity restrictions are then imposed on the adjoint angular flux at the interfaces of contiguous regions. Once a set of N nodes and weights $\{\mu_i, w_i\}$ of a quadrature scheme are fixed for the interval $[0, 1]$, the angular dependence of the homogeneous equation is discretized in the directions $\mu = \pm\mu_i$ as

$$\mp\mu_i \frac{d}{dz}\psi_h^\dagger(z, \pm\mu_i) + \sigma\psi_h^\dagger(z, \pm\mu_i) = \frac{c}{2}\sum_{l=0}^{L}\beta_l P_l(\mu_i) d_l(z) \tag{16a}$$

with

$$d_l(z) = \sum_{k=1}^{N} w_k P_l(\mu_k)\left[\psi_h^\dagger(z, \mu_k) + (-1)^l \psi_h^\dagger(z, -\mu_k)\right]. \tag{16b}$$

Moving on, spectral solutions in the form

$$\psi_h^\dagger(z, \pm\mu_i) = \phi(\nu, \mu_i)e^{-z/\nu} \tag{17}$$

are sought. After a series of algebraic operations carefully described in Pazinatto et. al. [2], the homogeneous solution to the adjoint transport equation is given by

$$\boldsymbol{\psi}_{\pm,h}^\dagger(z) = \sum_{j=1}^{N}\left[a_j\boldsymbol{\phi}_\pm(\nu_j)e^{-z/\nu_j} + b_j\boldsymbol{\phi}_\mp(\nu_j)e^{-(z_0-z)/\nu_j}\right], \tag{18}$$

where $\boldsymbol{\psi}_{\pm,h}^\dagger(z) = \left[\psi_h^\dagger(z, \pm\mu_i)\right] \in \mathbb{R}^N$ and $\boldsymbol{\phi}_\pm(\nu) = [\phi(\nu, \pm\mu_i)] \in \mathbb{R}^N$ with eigenfunctions defined by

$$\boldsymbol{\phi}_\pm(\nu) = \frac{1}{2}\boldsymbol{M}^{-1}\left(\boldsymbol{I} \mp \nu\boldsymbol{B}_+\right)\boldsymbol{x}, \tag{19a}$$

with $\boldsymbol{M} = \operatorname{diag}(\mu_i) \in \mathbb{R}^{N\times N}$, where $\boldsymbol{x} \in \mathbb{R}^N$ and $\nu > 0$ are such that

$$\boldsymbol{B}_-\boldsymbol{B}_+\boldsymbol{x} = \frac{1}{\nu^2}\boldsymbol{x}, \tag{19b}$$

with $\boldsymbol{B}_\pm \in \mathbb{R}^{N\times N}$ written as

$$\boldsymbol{B}_{+} = \left(\sigma \boldsymbol{I} - \frac{c}{2}\sum_{l=0}^{L}\beta_l \boldsymbol{\Pi}_l \boldsymbol{\Pi}_l^T \boldsymbol{W}[1+(-1)^l]\right)\boldsymbol{M}^{-1} \tag{19c}$$

and

$$\boldsymbol{B}_{-} = \left(\sigma \boldsymbol{I} - \frac{c}{2}\sum_{l=0}^{L}\beta_l \boldsymbol{\Pi}_l \boldsymbol{\Pi}_l^T \boldsymbol{W}[1-(-1)^l]\right)\boldsymbol{M}^{-1} \tag{19d}$$

where $\boldsymbol{\Pi}_l = [P_l(\mu_i)] \in \mathbb{R}^N$ and $\boldsymbol{W} = \text{diag}(w_i) \in \mathbb{R}^{N\times N}$.

For the special case where $S^\dagger$ is a constant source, a particular solution is written as

$$\psi_p^\dagger(z,\mu) = \frac{S^\dagger}{\sigma - c\beta_0} \tag{20}$$

and can be easily verified by direct substitution into the adjoint transport equation. It is noted however that in order to apply this particular solution, the domain must be divided such that there are no regions with more than one detector in order to deal with possible discontinuities on the particular solution.

On the other hand, if $S^\dagger$ is a non-constant source, a systematic approach is obtained by the use of Green's functions in infinite medium as derived in [7] by Barichello and Siewert, and latter extended to the adjoint transport equation. This particular solution is expressed in terms of the eigenfunctions $\boldsymbol{\phi}_\pm$ defined in Equation (19a) and is written as

$$\boldsymbol{\psi}_{\pm,p}^\dagger(z) = \sum_{j=1}^{N}\left[a_j(z)\boldsymbol{\phi}_\pm(\nu_j) + b_j(z)\boldsymbol{\phi}_\mp(\nu_j)\right] \tag{21}$$

where, for an isotropically defined source $S^\dagger$,

$$a_j(z) = c_j \int_0^z S^\dagger(z')e^{-(z-z')/\nu_j}dz' \tag{22a}$$

and

$$b_j(z) = c_j \int_z^{z_0} S^\dagger(z')e^{-(z'-z)/\nu_j}dz' \tag{22b}$$

with

$$c_j = -\frac{\displaystyle\sum_{i=1}^{N} w_i\left[\phi(\nu_j,\mu_i) + \phi(\nu_j,-\mu_i)\right]}{\displaystyle\sum_{i=1}^{N} w_i\mu_i\left[\phi(\nu_j,\mu_i)^2 - \phi(\nu_j,-\mu_i)^2\right]}. \tag{22c}$$

It should be stressed that this particular solution formulation allows to deal with source terms defined as piecewise functions, without imposing any restrictions on the domain division, which reduces the order of the linear system in comparison with the treatment mentioned previously for the constant case. However, the evaluation of the spatial integrals in Equation (22) might be costly if they are to be approximated by a quadrature scheme, an inexistent problem if analytical expression for the integrals are available.

V. COMPUTATIONAL ASPECTS AND NUMERICAL RESULTS

All tests were performed on a machine equipped with an Intel Core i5-4670 processor with 16 GiB of RAM. The minimization of the objective function defined in Equation (15) was performed by the non-negative least squares *nnls* subroutine, available at Netlib[1]. As a first test problem, the reconstruction of a polynomial source

$$S(z) = -\frac{z^2}{150}(z-10) \tag{23}$$

is considered for $z_0 = 10$. The physical parameters are set as $c = 0.99$, $\sigma = 1$, $\beta_0 = 1$, $\beta_1 = 9/4$, $\beta_2 = 25/12$, $\beta_3 = 7/6$, $\beta_4 = 9/22$, $\beta_5 = 1/12$ and $\beta_6 = 1/132$ [2]. It is also assumed that there is no incoming flux at the boundaries $z = 0$ and $z = 10$.

A set of ten neutral particle detectors are uniformly distributed within the physical domain with absorption cross-sections

$$\sigma_{d,i} = \begin{cases} 0.1, & z \in [0.4+i-1, 0.6+i-1], \\ 0.0, & \text{otherwise,} \end{cases} \tag{24}$$

with $i = 1,\ldots,10$. For each detector, a reading $r_{m,i}$ is computed by Equation (4) using the solution of the transport equation $\mathcal{L}\psi = S$ obtained by the ADO method with $N = 4$, thereafter, white noise is applied to the readings in order to generate 5000 different tests to the problem. Figure (1) shows the distribution of the maximum error imposed on the readings $r_{m,i}$.

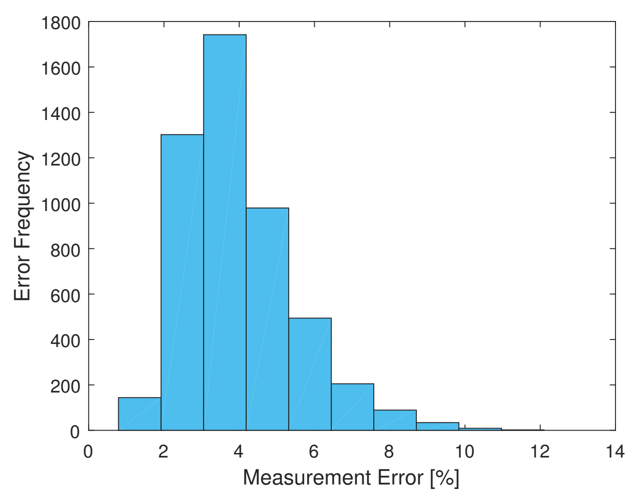

Fig. 1. Measurement errors imposed on the readings $r_{m,i}$.

For the first test, a partition

$$[0,10] = \bigcup_{j=1}^{10}[j-1, j] \tag{25}$$

is considered in Equation (14) to define the basis functions. In Figure (2), the dashed line represents the true source S defined in Equation (23) and the solid lines are the reconstruction $\hat{S}$

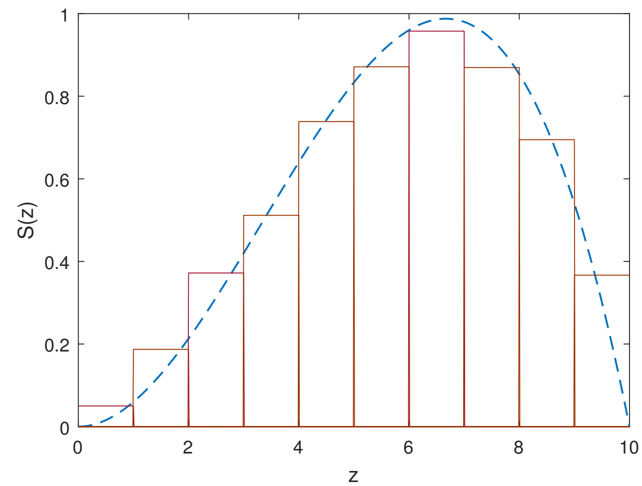

Fig. 2. Reconstruction using partition $[0, 10] = \bigcup_{j=1}^{10} [j-1, j]$. Dashed line is the true source S and solid lines represent the reconstruction $\hat{S}$.

of minimal relative error from all the reconstructions. As the graph in Figure (2) indicates, the reconstruction process was able to recover the shape of the source of neutral particles S.

Next, the transport equation $\mathcal{L}\hat{\psi} = \hat{S}$ is solved in order to compute readings $\hat{r}_{m,i}$ with the reconstructed source $\hat{S}$. Relative errors between the noisy free measurements and the reconstructions were computed. Figure (3) indicates a be-

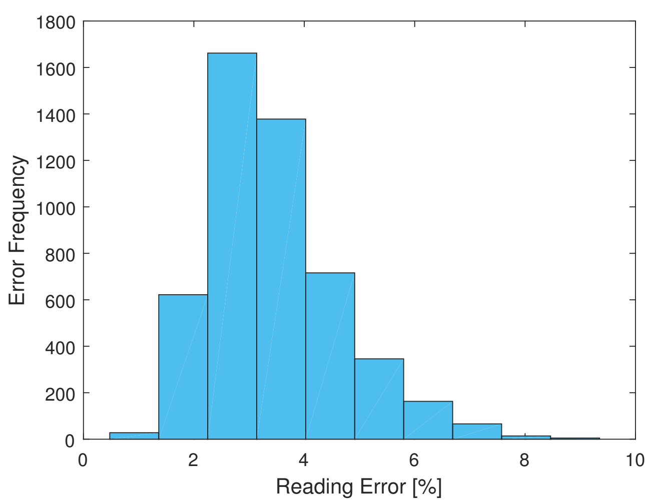

Fig. 3. Relative errors on the reconstructed reading $\hat{r}_{m,i}$ using partition the $[0, 10] = \bigcup_{j=1}^{10} [j-1, j]$.

havior similar between the error in the measurements and the reconstruction error. It is also highlighted that the maximum value computed to the Tikhonov's regularization parameter was 0.0680.

[1]http://www.netlib.org/, last accessed in 9/17/2016.

As a second reconstruction test, a partition

$$[0, 10] = \bigcup_{j=1}^{20} [0.5(j-1), 0.5j] \qquad (26)$$

is considered in Equation (14). Similarly to the previous reconstruction, the graph in Figure (4) indicates that the reconstruction process was able to recover the shape of the source of neutral particles S.

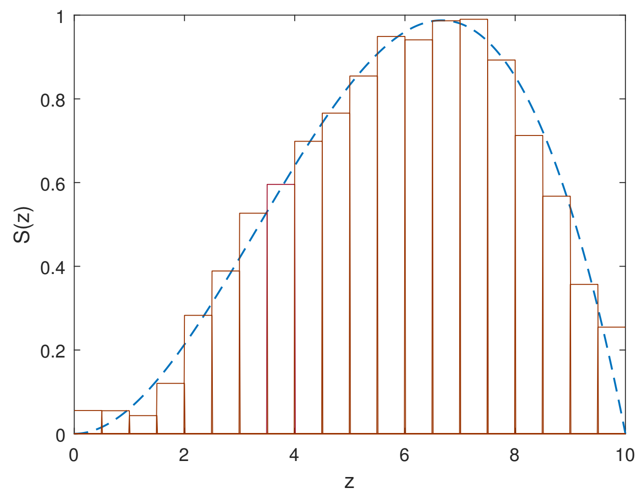

Fig. 4. Reconstruction using partition the $[0, 10] = \bigcup_{j=1}^{20} [0.5(j-1), 0.5j]$. Dashed line is the true source S and solid lines represent the reconstruction $\hat{S}$.

After the numerical evaluation of the transport equation using the reconstructed source $\hat{S}$, the relative errors in Figure (5) were found to be similar to the measurement errors in Figure (1) and the relative reconstruction for the previous test case in Figure (3). The maximum value computed to the Tikhonov's regularization parameter was 0.0472, slightly inferior to the previous reconstruction test.

As a third test problem, it is considered the reconstruction of a localized source piecewisely defined for $z \in [0, 30]$ by

$$S(z) = \begin{cases} 0.75, & z \in [17, 20), \\ 1.00, & z \in [20, 24), \\ 0.25, & z \in [24, 26], \\ 0.00, & \text{otherwise.} \end{cases} \qquad (27)$$

The particles are assumed to be isotropically migrating within the slab, a medium with physical parameters set as $c = 0.3$, $\sigma = 1$ and $\beta_0 = 1$. As before, it is also assumed that there is no incoming flux at the boundaries $z = 0$ and $z = 30$.

At this time, a set of sixty neutral particle detectors are uniformly distributed within the physical domain, with absorption cross section

$$\sigma_{d,i} = \begin{cases} 0.1, & z \in [(2j - 11/10)/4, (2j - 9/10)/4], \\ 0.0, & \text{otherwise,} \end{cases} \qquad (28)$$

with $i = 1, \ldots, 60$. Just as before, for each detector, a reading $r_{m,i}$ is computed by Equation (4) and, thereafter, white noise

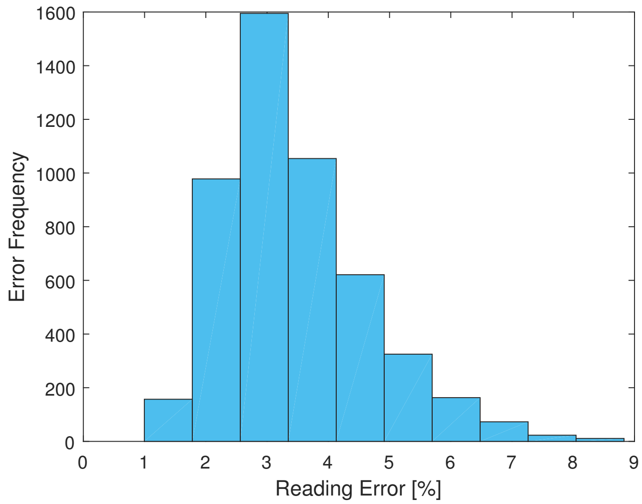

Fig. 5. Relative errors on the reconstructed reading $\hat{r}_{m,i}$ using partition $[0, 10] = \bigcup_{j=1}^{20} [0.5(j-1), 0.5j]$.

were applied to the readings in order to generate 5000 different tests to the problem. Figure (6) shows the distribution of the maximum error imposed on the readings $r_{m,i}$.

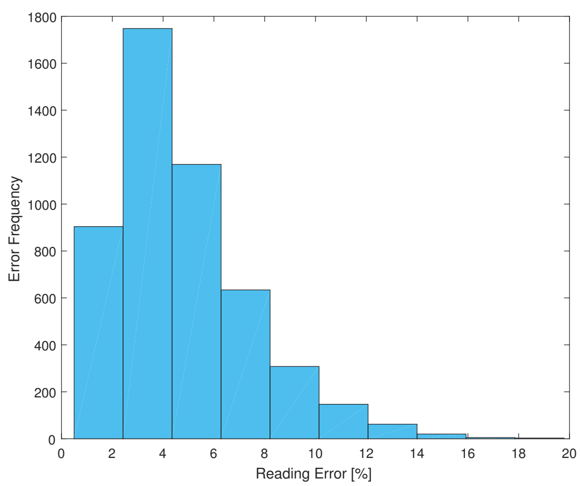

Fig. 6. Measurement errors imposed on the readings $r_{m,i}$.

For the reconstruction, a partition

$$[0, 30] = \bigcup_{j=1}^{60} [0.5(j-1), 0.5j] \tag{29}$$

is considered in Equation (14). In Figure (7), the dashed line represents the true source S defined in Equation (23) and the solid lines are the reconstruction $\hat{S}$ of minimal relative error from all the reconstructions.

The transport equation is evaluated using the reconstructed source $\hat{S}$ in order to calculate the relative errors between the exact measurements and the noisy ones. Figure (8) exhibits the maximum relative errors among the sixty measurements for all 5000 tests. The errors were found to be inferior

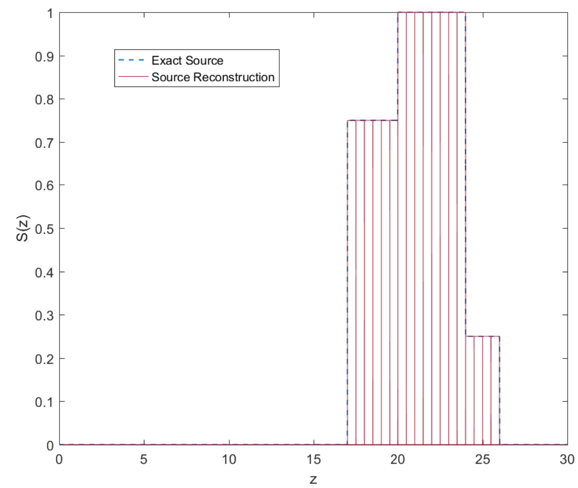

Fig. 7. Reconstruction using partition $[0, 30] = \bigcup_{j=1}^{60} [0.5(j-1), 0.5j]$. Dashed line is the true source S and solid lines represent the reconstruction $\hat{S}$.

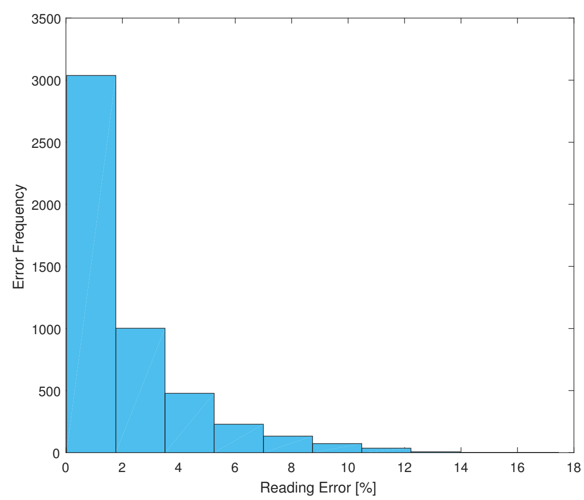

Fig. 8. Relative errors on the reconstructed reading $\hat{r}_{m,i}$ using partition $[0, 30] = \bigcup_{j=1}^{60} [0.5(j-1), 0.5j]$.

than the noise added to the measurements as Figure (6) indicates. For this test problem, the maximum value among the Tikhonov's regularization parameters was 0.1221, a higher value than the ones presented on the previous test problems.

According to Equation (28), 60 particles detectors are currently distributed uniformly within the slab, where 18 of these detectors are within the positive source range, $z \in [17, 26]$. As a fourth and final test, all of these detectors are removed with the exception of the ones defined in Equation (28) with $i = 38, 41, 46$ and 51, resulting on an underdetermined system in Equation (13). The distribution of the maximum error added to the readings $r_{m,i}$ is shown in Figure (9).

For each reconstruction, the transport equation is evalu-

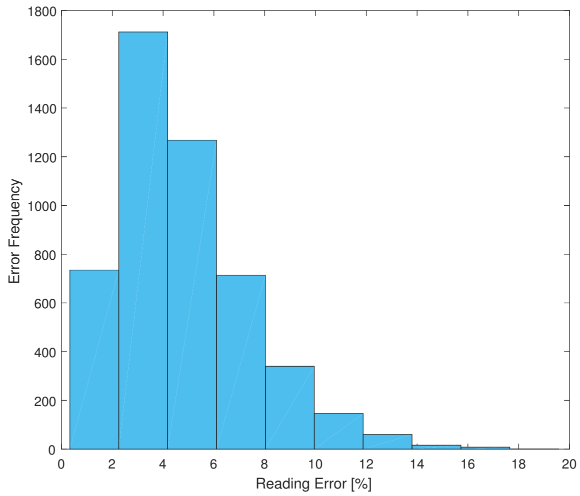

Fig. 9. Measurement errors imposed on the readings $r_{m,i}$.

ated with the reconstructed source and the detectors readings are computed. Figure (10) shows the maximum relative errors among all detectors between the readings calculated using the reconstructions and the original source. The maximum value of the regularization parameter in Equation (15) was the same as before, 0.1221.

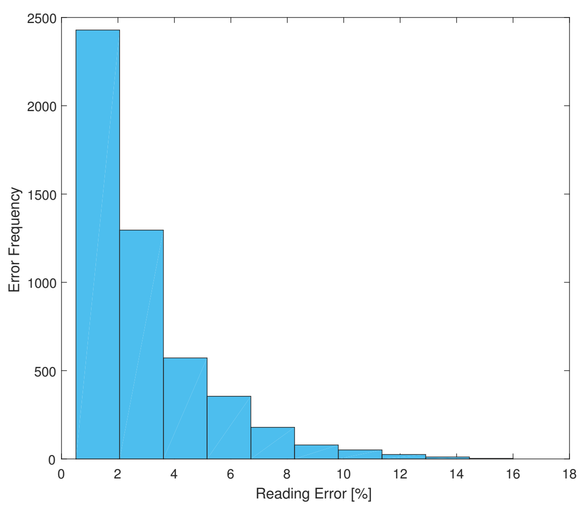

Fig. 10. Relative errors on the reconstructed reading $\hat{r}_{m,i}$ using partition $[0, 30] = \bigcup_{j=1}^{60} [0.5(j-1), 0.5j]$.

VI. DISCUSSION

The *Analytical Discrete Ordinates* method was successfully applied in a simple source reconstruction model problem, yielding good results in the sense that errors on the estimated measurements were found slightly inferior to the noise added to the real readings. Moreover, the first test problem took an average of 6.9×10^{-4} seconds per inversion. For the second test problem, an average of 1.2×10^{-3} seconds was required per inversion. The third and fourth test problems took an average of 9.8×10^{-3} and 8.8×10^{-3} seconds per inversion. The ADO formulation is still open to be tested against probabilistic approaches to the solution of the adjoint transport problem. Currently additional tests related to localized sources and alternative forms of errors are being performed as well as the inclusion of energy dependence in the model problem .

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