A Comparison of Three Quadrature Schemes for Discrete-Ordinates Calculations of Neutral Particle Transport in Ducts

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Abstract

The use of three different quadrature schemes in discrete-ordinates calculations of neutral particle transport in ducts of arbitrary but uniform cross-sectional geometry is studied. The considered schemes are: (i) the single-quadrature scheme defined by the standard Gauss-Chebyshev quadrature generated by the measure $(1-\mu^2)^{1/2}d\mu$ on $[-1,1]$, (ii) the double-quadrature scheme based on the nonstandard Gaussian quadrature generated by the measure $(1-\mu^2)^{1/2}d\mu$ on $[0,1]$ and its counterpart on $[-1,0]$, and (iii) the double-quadrature scheme based on the standard Gauss-Legendre quadrature mapped onto $[-1,0]$ and $[0,1]$. To implement the discrete-ordinates method, an approximate model of transport in ducts derived from a weighted residual procedure with two basis and two weight functions is adopted. The main conclusion of this work is that the double-quadrature scheme based on the nonstandard measure is the best of the three. However, for those who do not wish to deal with the special techniques of the constructive theory of orthogonal polynomials that are required to generate this scheme, the standard double Gauss-Legendre scheme constitutes a viable alternative.

1 Introduction

The problem of neutral-particle transport in an evacuated duct with a purely scattering wall is known in kinetic theory as free molecular flow. As a classical problem in the field, this problem has been studied since early times (Loeb, 1934); even so, new studies and approaches continue to be reported in the literature along the years (Davis, 1960; Garelis, 1973; Fustoss, 1981).

Some years ago, Prinja and Pomraning (Prinja, 1984) contributed to a renewal of the interest in the duct problem from the perspective of controlled-fusion research. As pointed out by these authors, the problem of quantifying the transport of energetic neutral particles, mainly atomic and molecular hydrogen isotopes and helium, in ducts of various cross-sectional geometries in tokamak devices is a very important one. Since the problem involves, in its most general form, multidimensional geometry, energy dependence and complicated wall scattering models, Monte Carlo simulation has been the preferred approach. However, Monte Carlo calculations are expensive, and this motivated Prinja and Pomraning to propose an approximate one-dimensional model for treating this problem. Their model includes the use of a standard multigroup approximation to treat the energy dependence of the problem, but the analysis in their paper was restricted to the space-angle treatment. Recently, the analysis has been extended to include energy dependence and a wall scattering model that allows the scattered particle to reappear at a different site on the wall than the original scattering site (Prinja, 1996).

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The approximate model developed by Prinja and Pomraning made it possible a reduction in the number of independent variables in the problem from five (three in space, two in angle) to two (one in space, one in angle). The essential idea of the model is to average the distance between wall collisions over the duct cross section and the azimuthal angle, and to interpret the resulting expression as a mean-free-path. As a result of this physical insight, a transport equation in the (z, μ) variables with an "interaction cross section" proportional to $(1-\mu^2)^{1/2}$ was obtained (Prinja, 1984).

At about the same time that the Prinja-Pomraning model was introduced, Larsen developed a more mathematically oriented way of deriving the model, by projecting the original transport equation and associated boundary conditions onto a (z, μ) subspace (Larsen, 1984). Larsen also showed that the Prinja-Pomraning model corresponds to the lowest order approximation in a hierarchy of approximations derived by a weighted residual procedure, but he did not pursue specific representations of basis and weight functions applicable to higher order models.

In a subsequent work (Larsen, 1986), Larsen, Malvagi and Pomraning were able to improve the precision of the one-dimensional model by considering the next order approximation in Larsen's hierarchy of approximations. As their model makes use of two basis functions, these authors called it the $N = 2$ model. The shape of the basis functions used to approximate the desired solution was suggested by the form of the angular flux in a duct subject to an isotropic source of particles emerging from the wall. In prescribing the weight functions against which the original transport equation and the associated boundary conditions were projected, two methods were considered: (i) the Galerkin procedure, based on weight functions that are the same as the basis functions for the problem; and (ii) a variational principle, based on weight functions that are the basis functions for the adjoint problem. In their sample calculations, Larsen, Malvagi and Pomraning used the discrete-ordinates method with a standard quadrature scheme (denoted as the *SS* scheme in this work) based on the Chebyshev polynomials of the second kind to compute reflection probabilities for semi-infinite and finite circular ducts and transmission probabilities for finite circular ducts. The discrete-ordinates equations were solved analytically for the case of a semi-infinite duct; for finite ducts, these equations were spatially discretized and solved numerically. Their converged numerical results compared well with reference results obtained from the Monte Carlo, integral equation and view factor approaches: a maximum error of $\sim 7\%$ was observed in the reflection and transmission probabilities for the test cases they considered and the computer time was only a fraction (typically $1/10$) of the Monte Carlo and view factor computer times. On the other hand, the $N = 1$ model of Prinja and Pomraning exhibited substantially larger errors that reached $\sim 400\%$ in the transmission probabilities for some test cases.

Recently, we devised an improved way (Garcia, 1999) of implementing the discrete-ordinates method for solving the finite duct problem in the $N = 2$ model. A reduction (in some cases, a factor of 10) in the number of ordinates used by Larsen, Malvagi and Pomraning to obtain converged results for the reflection and transmission probabilities for circular ducts was achieved by decomposing the problem into uncollided and collided problems prior to using the discrete-ordinates approximation, and by using a double-quadrature scheme (denoted here as the *DN* scheme) based on the nonstandard half-range quadrature generated by the measure $(1-\mu^2)^{1/2}d\mu$ on $[0, 1]$ (and its counterpart on $[-1, 0]$) to solve the collided problem.

In this work, we study the alternative of using a double-quadrature scheme (denoted as the *DS* scheme) based on the standard Gauss-Legendre quadrature mapped onto $[-1, 0]$ and $[0, 1]$ to solve the collided problem in the discrete-ordinates approximation to the $N = 2$ model. The idea of trying the Gauss-Legendre scheme for this problem was suggested by Siewert (Siewert, 1998), who has successfully used convenient mappings of this quadrature to develop discrete-ordinates solutions for various problems defined by transport equations with unconventional scattering terms (Barichello, 1999; Siewert, 1999a; Siewert, 1999b).

2 The model

Following Larsen, Malvagi and Pomraning (Larsen, 1986), we note that the particle distribution function $\Psi(\mathbf{r}, \boldsymbol{\Omega})$ in an evacuated duct of cross-sectional area A and length Z must satisfy the transport equation

$$\boldsymbol{\Omega} \cdot \nabla\Psi(\mathbf{r}, \boldsymbol{\Omega}) = 0, \tag{1}$$

where $\mathbf{r}$ and $\boldsymbol{\Omega}$ are, respectively, the position and the direction of particle motion, and can be expressed in Cartesian coordinates as $\mathbf{r} = (x, y, z)$ and $\boldsymbol{\Omega} = \left[(1 - \mu^2)^{1/2} \cos\varphi, (1 - \mu^2)^{1/2} \sin\varphi, \mu\right]$. The region in space where Eq. (1) is valid consists of the interior of the duct, which is specified by $R = [(x, y) \mid h(x, y) < 0]$ and $0 < z < Z$. Here, $h(x, y)$ is a function that describes the duct cross-sectional shape, so that $\partial R = [(x, y) \mid h(x, y) = 0]$ denotes the contour of the duct inner wall. With these definitions, the duct cross-sectional area and the duct perimeter are given, respectively, by $A = \int_R dxdy$ and $L = \int_{\partial R} ds$, where ds is an elementary arc length.

In regard to the boundary conditions needed to complete the formulation of the problem, prescribed incident particle distributions are assumed at the duct ends, i.e.

$$\Psi(x, y, 0, \mu, \varphi) = F(x, y, \mu, \varphi) \tag{2a}$$

and

$$\Psi(x, y, Z, -\mu, \varphi) = G(x, y, \mu, \varphi), \tag{2b}$$

for $(x, y) \in R$, $0 < \mu \leq 1$ and $0 \leq \varphi \leq 2\pi$. In addition, the duct inner wall is characterized by partial isotropic reflection, written in general form as

$$-\boldsymbol{\Omega} \cdot \mathbf{n}\Psi(\mathbf{r}, \boldsymbol{\Omega}) = \int_{\boldsymbol{\Omega}' \cdot \mathbf{n} > 0} p(\mathbf{r}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega})\Psi(\mathbf{r}, \boldsymbol{\Omega}')d\Omega', \tag{3}$$

for $(x, y) \in \partial R$, $0 < z < Z$ and $\boldsymbol{\Omega} \cdot \mathbf{n} < 0$, where

$$p(\mathbf{r}, \boldsymbol{\Omega}' \to \boldsymbol{\Omega}) = -\left(\frac{c}{\pi}\right)(\boldsymbol{\Omega} \cdot \mathbf{n})(\boldsymbol{\Omega}' \cdot \mathbf{n}), \tag{4}$$

$\mathbf{n}$ denotes the unit outward normal vector at position $\mathbf{r}$ on ∂R, and c is the probability that a particle striking the inner wall will be reflected towards the duct interior.

In the $N = 2$ model discussed in detail by Larsen, Malvagi and Pomraning (Larsen, 1986), the particle distribution function $\Psi(x, y, z, \mu, \varphi)$ is approximated in terms of the prescribed basis functions $\alpha_j(x, y, \varphi)$, $j = 1$ and 2, as

$$\Psi(x, y, z, \mu, \varphi) \approx \Psi_1(z, \mu)\alpha_1(x, y, \varphi) + \Psi_2(z, \mu)\alpha_2(x, y, \varphi), \tag{5}$$

and a weighted residual procedure (Galerkin or variational) is used to deduce two coupled transport equations for the coefficients of the approximation $\Psi_j(z,\mu)$, $j = 1$ and 2, and their corresponding boundary conditions. The resulting transport equations can be written in matrix form as

$$\mu\frac{\partial}{\partial z}\mathbf{\Psi}(z,\mu) + (1-\mu^2)^{1/2}\mathbf{A}\mathbf{\Psi}(z,\mu) = \frac{2c}{\pi}(1-\mu^2)^{1/2}\mathbf{B}\int_{-1}^{1}(1-\mu'^2)^{1/2}\mathbf{\Psi}(z,\mu')d\mu', \tag{6}$$

for $0 < z < Z$ and $-1 \le \mu \le 1$, and the boundary conditions as

$$\mathbf{\Psi}(0,\mu) = \mathbf{F}(\mu) \tag{7a}$$

and

$$\mathbf{\Psi}(Z,-\mu) = \mathbf{G}(\mu), \tag{7b}$$

for $0 < \mu \le 1$. Here $\mathbf{\Psi}(z,\mu)$ is a column vector of two components, the unknown coefficients $\Psi_j(z,\mu)$, $j = 1$ and 2, in the approximate representation expressed by Eq. (5), $\mathbf{A}$ and $\mathbf{B}$ are 2×2 full matrices that depend on the duct cross-sectional geometry and on the prescriptions of the basis and weight functions (Larsen, 1986) and the vectors $\mathbf{F}(\mu)$ and $\mathbf{G}(\mu)$ have, respectively, components $F_j(\mu)$ and $G_j(\mu)$, $j = 1$ and 2, that are given by

$$F_j(\mu) = \frac{1}{2\pi A}\int_R\int_0^{2\pi}\beta_j(x,y,\varphi)F(x,y,\mu,\varphi)d\varphi dx dy \tag{8a}$$

and

$$G_j(\mu) = \frac{1}{2\pi A}\int_R\int_0^{2\pi}\beta_j(x,y,\varphi)G(x,y,\mu,\varphi)d\varphi dx dy, \tag{8b}$$

where $\beta_j(x,y,\varphi)$, $j = 1$ and 2, are the prescribed weight functions.

3 Decomposition into uncollided and collided problems

The desired solution to the problem formulated by Eqs. (6) and (7) can be split into uncollided and collided components as

$$\mathbf{\Psi}(z,\mu) = \mathbf{\Psi}_0(z,\mu) + \mathbf{\Psi}_*(z,\mu). \tag{9}$$

Here the uncollided component of the solution, $\mathbf{\Psi}_0(z,\mu)$, is defined so that it satisfies Eq. (6) for $c = 0$ and Eqs. (7), i.e.

$$\mu\frac{\partial}{\partial z}\mathbf{\Psi}_0(z,\mu) + (1-\mu^2)^{1/2}\mathbf{A}\mathbf{\Psi}_0(z,\mu) = 0, \tag{10}$$

for $0 < z < Z$ and $-1 \le \mu \le 1$, and

$$\mathbf{\Psi}_0(0,\mu) = \mathbf{F}(\mu) \tag{11a}$$

and

$$\mathbf{\Psi}_0(Z,-\mu) = \mathbf{G}(\mu), \tag{11b}$$

for $0 < \mu \leq 1$, while the collided component, $\mathbf{\Psi}_*(z,\mu)$, must satisfy

$$\mu\frac{\partial}{\partial z}\mathbf{\Psi}_*(z,\mu) + (1-\mu^2)^{1/2}\mathbf{A}\mathbf{\Psi}_*(z,\mu) = \frac{2c}{\pi}(1-\mu^2)^{1/2}\mathbf{B}\int_{-1}^{1}(1-\mu'^2)^{1/2}\mathbf{\Psi}_*(z,\mu')d\mu' + \mathbf{Q}(z,\mu), \tag{12}$$

for $0 < z < Z$ and $-1 \leq \mu \leq 1$, and the boundary conditions

$$\mathbf{\Psi}_*(0,\mu) = \mathbf{\Psi}_*(Z,-\mu) = \mathbf{0} \tag{13}$$

for $0 < \mu \leq 1$. We note that in Eq. (12) the first-collision source $\mathbf{Q}(z,\mu)$ is expressed as

$$\mathbf{Q}(z,\mu) = \frac{2c}{\pi}(1-\mu^2)^{1/2}\mathbf{B}\int_{-1}^{1}(1-\mu'^2)^{1/2}\mathbf{\Psi}_0(z,\mu')d\mu', \tag{14}$$

and becomes explicitly known once the uncollided problem is solved.

In regard to the uncollided problem, a diagonalization procedure was used (Garcia, 1999) to reduce this problem to a decoupled "two-group" problem for which an analytical solution can be readily found. The resulting uncollided solution can be written as (Garcia, 1999)

$$\mathbf{\Psi}_0(z,\mu) = \left[\mathbf{U}_{12}e^{-\lambda_1(1-\mu^2)^{1/2}z/\mu} + \mathbf{U}_{21}e^{-\lambda_2(1-\mu^2)^{1/2}z/\mu}\right]\mathbf{F}(\mu) \tag{15a}$$

and

$$\mathbf{\Psi}_0(z,-\mu) = \left[\mathbf{U}_{12}e^{-\lambda_1(1-\mu^2)^{1/2}(Z-z)/\mu} + \mathbf{U}_{21}e^{-\lambda_2(1-\mu^2)^{1/2}(Z-z)/\mu}\right]\mathbf{G}(\mu), \tag{15b}$$

for $0 \leq z \leq Z$ and $0 < \mu \leq 1$, where λ_1 and λ_2 are the eigenvalues of $\mathbf{A}$ and, for $\lambda_1 \neq \lambda_2$,

$$\mathbf{U}_{ij} = \frac{1}{\lambda_i - \lambda_j}\begin{pmatrix} \lambda_i - a_{22} & -(\lambda_i - a_{22})(\lambda_j - a_{22})/a_{21} \\ a_{21} & -(\lambda_j - a_{22}) \end{pmatrix}, \tag{16}$$

with a_{ij} denoting the (i,j) element of $\mathbf{A}$. We note that an alternative representation of $\mathbf{U}_{ij}$ is available for treating the degenerate case $\lambda_1 = \lambda_2$, and that, to avoid the need of using complex arithmetic in the calculation, Eqs. (15) were reformulated in terms of real quantities for the case where the eigenvalues of $\mathbf{A}$ appear as a complex conjugate pair (Garcia, 1999).

4 A numerical discrete-ordinates solution for the collided problem

If the spatial dependence of Eq. (12) is discretized according to a spatial mesh defined by the points z_k, $k = 0,1,\ldots,K$, with $z_0 = 0$ and $z_K = Z$, and the angular dependence according to a set of discrete directions μ_i, $i = 1,2,\ldots,M$, chosen as the nodes of the quadrature of order M used to approximate the integral in this equation, then the fully numerical discrete-ordinates version of the collided problem defined by Eqs. (12) and (13) can be written as the set of linear algebraic equations, for $k = 1,2,\ldots,K$ and $i = 1,2,\ldots,M$,

$$\frac{\mu_i}{\Delta_k}\left[\mathbf{\Psi}_{k,i} - \mathbf{\Psi}_{k-1,i}\right] + (1-\mu_i^2)^{1/2}\mathbf{A}\bar{\mathbf{\Psi}}_{k,i} = \frac{2c}{\pi}(1-\mu_i^2)^{1/2}\mathbf{B}\sum_{j=1}^{M}\omega_j W_j \bar{\mathbf{\Psi}}_{k,j} + \bar{\mathbf{Q}}_{k,i}, \tag{17}$$

subject to the boundary conditions

$$\mathbf{\Psi}_{0,i} = \mathbf{0}, \tag{18a}$$

for the values of i such that $\mu_i > 0$, and

$$\mathbf{\Psi}_{K,i} = \mathbf{0}, \tag{18b}$$

for the values of i such that $\mu_i < 0$. Here $\Delta_k = z_k - z_{k-1}$, $\mathbf{\Psi}_{k,i} = \mathbf{\Psi}_*(z_k, \mu_i)$ is the vector of coefficients for the *collided* angular flux at the mesh edge z_k along the ordinate μ_i,

$$\bar{\mathbf{\Psi}}_{k,i} = \frac{1}{\Delta_k}\int_{z_{k-1}}^{z_k} \mathbf{\Psi}_*(z, \mu_i)dz \tag{19}$$

is the vector of mesh-averaged coefficients for the *collided* angular flux along the ordinate μ_i,

$$\bar{\mathbf{Q}}_{k,i} = \frac{1}{\Delta_k}\int_{z_{k-1}}^{z_k} \mathbf{Q}(z, \mu_i)dz \tag{20}$$

is the vector of mesh-averaged sources along the ordinate μ_i, $\{\omega_j\}$ are the quadrature weights, and

$$W_j = \begin{cases} 1 & \text{, for the } SS \text{ and the } DN \text{ quadrature schemes,} \\ (1-\mu_j^2)^{1/2} & \text{, for the } DS \text{ quadrature scheme.} \end{cases} \tag{21}$$

Looking at Eqs. (17) and (18), we can conclude that we have only $2KM$ equations for the $4KM$ unknowns ($2KM$ edge quantities and $2KM$ mesh-averaged quantities). A simple way of obtaining the $2KM$ complementary relations needed to match the number of equations to the number of unknowns is to use the "diamond-difference" approximation (Bell, 1970)

$$\bar{\mathbf{\Psi}}_{k,i} = \frac{1}{2}\left(\mathbf{\Psi}_{k-1,i} + \mathbf{\Psi}_{k,i}\right) \tag{22}$$

for $k = 1, 2, \ldots, K$ and $i = 1, 2, \ldots, M$. Equation (22) simply approximates the mesh-averaged coefficient vector as the average between the coefficient vectors at the edges of the mesh, and thus we can use this equation to eliminate the mesh-averaged coefficient vectors in Eq. (17), in analogy with the procedure adopted for the conventional scalar case (Bell, 1970). Applying a diagonalization procedure similar to the one used to find the solution for the uncollided problem in Sec. 3, we can write the resulting equation as (Garcia, 1999)

$$\mathbf{\Psi}_{k,i} = \left[2\mathbf{C}_{ik} - \mathbf{I}\right]\mathbf{\Psi}_{k-1,i} + \mathbf{C}_{ik}\mathbf{S}_{k,i}, \tag{23a}$$

for the values of i such that $\mu_i > 0$, and

$$\mathbf{\Psi}_{k-1,i} = \left[2\mathbf{C}_{ik} - \mathbf{I}\right]\mathbf{\Psi}_{k,i} + \mathbf{C}_{ik}\mathbf{S}_{k,i}, \tag{23b}$$

for the values of i such that $\mu_i < 0$. In these equations, we use the definitions

$$\mathbf{S}_{k,i} = \frac{\Delta_k}{|\mu_i|}\left[\frac{c}{\pi}(1-\mu_i^2)^{1/2}\mathbf{B}\sum_{j=1}^{M}\omega_j W_j\left(\mathbf{\Psi}_{k-1,j} + \mathbf{\Psi}_{k,j}\right) + \bar{\mathbf{Q}}_{k,i}\right] \tag{24}$$

and

$$\mathbf{C}_{ik} = \frac{1}{(1+s_{ik}\lambda_1)(1+s_{ik}\lambda_2)} \begin{pmatrix} 1+s_{ik}a_{22} & s_{ik}(\lambda_1-a_{22})(\lambda_2-a_{22})/a_{21} \\ -s_{ik}a_{21} & 1+s_{ik}(\lambda_1+\lambda_2-a_{22}) \end{pmatrix}, \tag{25}$$

with $s_{ik} = (1-\mu_i^2)^{1/2}\Delta_k/(2|\mu_i|)$. Again, we consider that Eq. (25) is in a convenient form only if the eigenvalues λ_1 and λ_2 are real. For the case where the eigenvalues appear as a complex pair, simple algebraic manipulations can be used to deduce an alternative representation for $\mathbf{C}_{ik}$, expressed in terms of real quantities only (Garcia, 1999).

To solve Eqs. (23), we have employed a standard sweep technique (Bell, 1970), where the boundary condition expressed by Eq. (18a) is used to initiate the application of Eq. (23a) across the mesh from left to right and the boundary condition expressed by Eq. (18b) is used to initiate the application of Eq. (23b) in the reverse direction. An initial value for the scattering component of the total source vector $\mathbf{S}_{k,i}$ defined by Eq. (24) is postulated (we used $\mathbf{0}$), and the process is considered converged when the computed components of $\mathbf{\Psi}_{k,i}$ do not differ (in relative terms) by more than a specified amount (10^{-8} was our choice), for all $k = 0, 1, \ldots, K$ and $i = 1, 2, \ldots, M$, in two successive sweeps.

5 Numerical results

In this section, we report the results of our investigation on the use of the *SS*, *DN* and *DS* quadrature schemes defined in the Introduction to solve the collided problem. We consider a test problem defined by an isotropic and uniform distribution of particles entering a circular duct of unitary radius at $z = 0$ (Larsen, 1986; Garcia, 1999). To begin, we report in Table 1 our converged results for the reflection (R) and transmission (T) probabilities

$$R = 2\int_0^1 \mu\Psi_1(0,-\mu)d\mu \tag{26a}$$

and

$$T = 2\int_0^1 \mu\Psi_1(Z,\mu)d\mu, \tag{26b}$$

for several values of the wall scattering probability (c) and of the duct length (Z) expressed in multiples of the duct radius. Assuming that the quadrature nodes have been ordered so that $1 > \mu_1 > \mu_2 > \cdots > \mu_M > -1$ and defining $m = M/2$, we can show that the discrete-ordinates results for the reflection and transmission probabilities can be expressed, for this problem, as

$$R = 2\sum_{i=m+1}^{M} \omega_i|\mu_i|(1-\mu_i^2)^{-1/2}W_i\Psi_{*1}(0,\mu_i) \tag{27a}$$

and

$$T = 2\int_0^1 \mu\Psi_{01}(Z,\mu)d\mu + 2\sum_{i=1}^{m}\omega_i\mu_i(1-\mu_i^2)^{-1/2}W_i\Psi_{*1}(Z,\mu_i), \tag{27b}$$

where $\Psi_{*1}(0,\mu_i)$, $i = m+1, m+2, \dots, M$, and $\Psi_{*1}(Z,\mu_i)i = 1, 2, \dots, m$ are the discrete-ordinates results for the first components of the *collided*-coefficient vectors $\Psi_*(0,\mu_i)$, $\mu_i < 0$, and $\Psi_*(Z,\mu_i)\mu_i > 0$ respectively, and $\Psi_{01}(Z,\mu)$ is the first component of the *uncollided*-coefficient vector given by Eq. (15a) for $z = Z$. We note that the results reported in Table 1 are based on the use of the *DN* quadrature scheme of order 256 (the other two schemes yielded the same converged results but at the expense of higher quadrature orders) and a uniform spatial discretization scheme with 640 mesh intervals for the cases where $Z = 1$ and 2560 mesh intervals for the cases where $Z = 20$. In addition, we note that we have found that the uncollided integral in Eq. (27b) can be accurately computed with the standard Gauss-Legendre quadrature of order 200 mapped onto [0, 1], for all of the test cases considered in this work.

Table 1: Converged reflection and transmission probabilities.

c	Z	R	T
0.2	1	4.6571(−2)	4.1431(−1)
0.2	20	5.4032(−2)	2.5011(−3)
0.5	1	1.3105(−1)	4.8516(−1)
0.5	20	1.6540(−1)	2.7229(−3)
0.8	1	2.4067(−1)	5.8096(−1)
0.8	20	3.6732(−1)	3.8224(−3)

Using the results in Table 1 as our reference, we show in Table 2 the relative percent deviations observed in the reflection and transmission probabilities obtained from discrete-ordinates calculations using the *SS*, *DN* and *DS* quadrature schemes in various orders. Uniform spatial discretization schemes with 80 mesh intervals for the cases where $Z = 1$ and 1280 mesh intervals for the cases where $Z = 20$ were used to generate these results. As can be seen in this table, the *DN* scheme introduced in our previous work (Garcia, 1999) converges, in general, more quickly than the other schemes, as M increases. On the other hand, the *DS* scheme yields, in most cases, the worst results in the lowest order of approximation ($M = 2$), but shows, especially for the reflection probability, a faster convergence rate than the *SS* scheme, as M increases.

6 Conclusions

Based on the numerical studies performed, we have concluded that, among the three quadrature schemes considered in this work for discrete-ordinates calculations in the $N = 2$ model of neutral particle transport in ducts, the *DN* scheme is the best. As this quadrature scheme is based on a nonstandard measure, and thus requires more laborious computational techniques (Gautschi, 1985) to be generated than the others, the *DS* scheme is a good option if one does not wish to deal with these techniques. Finally, it should be made clear that the amount of computer time needed to generate these quadratures is not at issue, since we have found that it is always negligible when compared with the amount of computer time needed to perform the rest of the calculation, which is essentially the same for all of the quadrature schemes studied.

Table 2: Relative percent deviations in the reflection and transmission probabilities computed with the *SS*, *DN* and *DS* quadrature schemes.

Duct Parameters		Quadrature Order	Percent Deviation in the Reflection Probability			Percent Deviation in the Transmission Probability		
c	Z	M	SS	DN	DS	SS	DN	DS
		2	22.1	13.0	35.1	2.3	0.71	3.6
		4	7.5	−0.48	1.2	0.24	−0.24	−0.19
		8	2.0	0.026	0.35	0.034	−0.002	0.039
0.2	1	16	0.59	0.0	0.043	0.022	0.0	0.005
		32	0.15	0.0	0.006	0.005	0.0	0.0
		64	0.039	0.0	0.0	0.0	0.0	0.0
		128	0.011	0.0	0.0	0.0	0.0	0.0
		2	14.8	2.3	27.7	−1.9	−2.1	−1.8
		4	5.9	−0.25	3.5	−1.7	−1.8	−1.6
		8	1.9	−0.024	0.52	−1.8	−1.6	−1.7
0.2	20	16	0.52	0.002	0.072	−1.4	−2.3	−1.8
		32	0.14	0.0	0.009	−0.048	−0.36	0.31
		64	0.033	0.0	0.0	0.0	0.0	0.044
		128	0.007	0.0	0.0	0.0	0.0	0.004
		2	14.4	8.9	27.3	3.9	1.2	7.0
		4	5.3	−0.36	1.5	0.42	−0.48	−0.26
		8	1.4	0.023	0.34	0.029	−0.002	0.095
0.5	1	16	0.42	0.0	0.046	0.031	0.0	0.012
		32	0.11	0.0	0.008	0.008	0.0	0.002
		64	0.023	0.0	0.0	0.002	0.0	0.0
		128	0.008	0.0	0.0	0.002	0.0	0.0
		2	8.8	−1.9	24.0	−7.4	−8.1	−6.7
		4	3.9	−0.65	3.6	−6.6	−7.0	−6.2
		8	1.3	−0.048	0.60	−7.0	−6.3	−6.6
0.5	20	16	0.36	0.0	0.085	−4.6	−8.0	−5.4
		32	0.091	0.0	0.012	−0.14	−1.1	1.0
		64	0.024	0.0	0.0	0.004	−0.004	0.14
		128	0.006	0.0	0.0	0.0	0.0	0.011
		2	5.7	4.3	18.6	2.8	0.76	7.7
		4	2.8	0.054	2.2	0.15	−0.50	0.065
		8	0.83	0.012	0.32	−0.069	0.0	0.14
0.8	1	16	0.23	0.0	0.046	0.002	0.0	0.017
		32	0.062	0.0	0.004	0.0	0.0	0.002
		64	0.017	0.0	0.0	0.0	0.0	0.0
		128	0.004	0.0	0.0	0.0	0.0	0.0
		2	2.3	−5.7	28.7	−28.6	−30.5	−22.2
		4	1.6	−1.2	4.2	−24.8	−26.5	−22.3
		8	0.63	−0.11	0.77	−22.7	−23.2	−21.0
0.8	20	16	0.19	−0.003	0.11	−8.8	−19.0	−8.1
		32	0.049	0.0	0.016	−0.21	−1.9	2.4
		64	0.014	0.0	0.003	0.013	0.010	0.28
		128	0.003	0.0	0.0	0.0	0.005	0.026

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