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EFFICIENT IMPLEMENTATION OF THE DISCRETE-ORDINATES METHOD FOR AN APPROXIMATE MODEL OF PARTICLE TRANSPORT IN DUCTS

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Abstract *Particle transport in ducts is, in general, a three-dimensional (3-D) problem and this makes it a big computational challenge. Usually, calculations are performed with the Monte Carlo method and are very time-consuming, especially for long ducts. A breakthrough in this field ocurred about 30 years ago, when Prinja and Pomraning introduced, in the context of controlled-fusion research, three approximate one-dimensional (1-D) models for studying neutral particle transport in ducts. In particular, the model that we study in this work is the best of the Prinja-Pomraning models, called "model 2" by these authors. In spite of being much more economical than Monte Carlo calculations, the model is not very accurate in certain situations. Fortunately, in the years that followed its introduction, model 2 of Prinja and Pomraning has been improved and widened its spectrum of applications to new research topics, such as light transport in ducts and propagation of sound in urban spaces. The model is based on a non-standard 1-D transport equation for a transverse and azimuthal average of the particle angular flux which is a function of only two variables: a spatial variable that gives the particle position along the duct axis and an angular variable that describes the direction of particle travel. In many works on this topic, the discrete-ordinates method has been used to discretize the angular variable and the spatial variable has also been discretized using finite differences. As a consequence of this purely numerical approach, the number of discrete ordinates (discretized values of the angular variable) needed for getting a reasonable precision in the solution of typical problems may reach or even exceed one hundred. In the present work, we show how a modern version of the discrete-ordinates method proposed by Barichello and Siewert can be adapted to solve the Prinja-Pomraning equation in a very efficient way. Since the spatial variable is not discretized in the approach of Barichello and Siewert, their method has been called analytical discrete-ordinates (ADO) method. In our studies, we have found that using only ten discrete ordinates in the ADO method we can get numerical results which are as precise as those that we get using one hundred discrete ordinates in the numerical version of the discrete-ordinates method. In conclusion, we have found that the savings in CPU time afforded by the ADO method are substantial: for three-digit precision, the ADO method is at least 20 times faster than the numerical discrete-ordinates method.*

1. INTRODUCTION

Particle transport in an evacuated duct with a non-absorbing wall is a classical problem in the kinetic theory of gases. In the study of gas flows, the flow regime where no particle collisions occur is known as free molecular flow. Since the duct problem, in its more general form, involves three-dimensional (3-D) geometry, energy and time dependence, and complicated wall scattering models, Monte Carlo simulation has been the preferred approach. However, Monte Carlo calculations are expensive, especially for long ducts. This motivated research on approximate models capable of reducing computation time with as low as possible accuracy loss.

In an important paper published in 1984, Prinja and Pomraning introduced three approximate one-dimensional (1-D) models of particle transport in ducts motivated by the study of schemes for removing neutral gas particles from tokamak devices [1]. The most successful of the simple models proposed by Prinja and Pomraning (model 2 of their work) is based on a non-standard transport equation for a transverse and azimuthal average of the particle angular flux which is a function of only two variables: a spatial variable that gives the particle position along the duct axis and an angular variable that describes the direction of particle travel. That model was put on firm mathematical grounds by Larsen [2], who also suggested ways of improving it. Some years later, 1-D models of higher order that improve on the accuracy of model 2 of Prinja and Pomraning were derived by Larsen, Malvagi, and Pomraning [3] and by Garcia, Ono, and Vieira [4], following Larsen's ideas [2]. Interestingly, some of these approximate models have been applied in recent years to new research topics such as light transport in ducts [5] and propagation of sound in urban spaces [6, 7].

In many works on the Prinja-Pomraning model and its improved versions, a purely numerical version of the discrete-ordinates method has been used where the angular variable is discretized by a quadrature rule and the spatial variable is discretized by finite differences [3, 4, 8–10]. A consequence of this approach is that the number of discrete ordinates (discretized values of the angular variable) needed for getting a reasonable accuracy in the solution for typical problems may reach or even exceed one hundred.

In this work, we show how a version of the discrete-ordinates method that was proposed by Barichello and Siewert [11] for solving radiative transfer problems can be adapted to solve the Prinja-Pomraning equation in a very efficient way. Since the spatial variable is not discretized and the discrete-ordinates equations can be solved analytically in the approach of Barichello and Siewert, their version of the discrete-ordinates method is known in the literature as analytical discrete-ordinates (ADO) method. To give an idea of the improvement afforded by the ADO method, we have found in our studies that using ten discrete ordinates in the ADO method we can get numerical results than are as precise as those that we only get using typically one hundred ordinates in the numerical version of the discrete-ordinates method.

2. FORMULATION OF THE PROBLEM

We consider in this work an evacuated, straight duct of length Z and uniform transverse cross section. Particles enter the duct by one of its ends (the *inlet*) and stream unimpeded until they collide with the duct wall or leave the duct by the other end. Upon collision with the wall, a particle can be absorbed or diffusely reflected. Particles that are not absorbed by the wall after one or more collisions end up leaving the duct by one of its ends. Mathematically, the physical process is described by a partial differential equation for the particle angular flux $\Psi(\mathbf{r}, \mathbf{\Omega})$ which can be written as [3]

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

Here, ∇ denotes the gradient operator and the independent variables $\mathbf{r}$ and $\mathbf{\Omega}$ are, respectively, the particle position and the unit vector in the direction of particle motion. In Cartesian coordinates, $\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$, $\mathbf{r} = (x, y, z)$ and $\mathbf{\Omega} = \left[(1-\mu^2)^{1/2}\cos\phi, (1-\mu^2)^{1/2}\sin\phi, \mu\right]$, where $\mu \in [-1, 1]$ is the cosine of the polar angle θ (measured with respect to the z-axis) and $\phi \in [0, 2\pi]$ is the azimuthal angle. 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 $0 < z < Z$, where $h(x, y)$ is a function that describes the duct cross-sectional shape. For example, in the case of a duct with circular cross section, $h(x, y) = x^2 + y^2 - \rho^2$, where ρ is the duct radius. 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 the differential arc length along the closed curve $\partial R = [(x, y) \mid h(x, y) = 0]$ which describes the contour of the duct wall in a plane perpendicular to the z-axis.

With regard to the boundary conditions needed to complete the formulation of the problem, we assume that particles are entering the duct end at $z = 0$ with a prescribed particle distribution $F(x, y, \mu, \phi)$ and that there are no particles entering the duct by the other end ($z = Z$). We thus write the boundary conditions at $z = 0$ and $z = Z$ as

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

and

$$\Psi(x, y, Z, -\mu, \phi) = 0, \tag{2b}$$

for $(x, y) \in R$, $\mu \in (0, 1]$, and $\phi \in [0, 2\pi]$. In addition, the duct wall is characterized by isotropic reflection, which can be written in general form as [3]

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

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

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

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

An approximate 1-D version of the problem defined by Eqs. (1) through (3) was first derived by Prinja and Pomraning [1], using an averaging process over the duct transverse cross section and the azimuthal angle that is described in detail in their work. The 1-D transport equation that is obtained from Eq. (1) can be written in the form [3]

$$\mu \frac{\partial}{\partial z} \psi(z, \mu) + \frac{L}{\pi A}(1-\mu^2)^{1/2} \psi(z, \mu) = \frac{2cL}{\pi^2 A}(1-\mu^2)^{1/2} \int_{-1}^{1} (1-\mu'^2)^{1/2} \psi(z, \mu') \mathrm{d}\mu, \tag{5}$$

for $z \in (0, Z)$ and $\mu \in [-1, 1]$. Here, the quantity $\psi(z, \mu)$ denotes the average of the angular flux $\Psi(x, y, z, \mu, \phi)$ over (x, y) and ϕ. Equation (5) is to be solved subject to the boundary conditions

$$\psi(0, \mu) = f(\mu) \tag{6a}$$

and

$$\psi(Z, -\mu) = 0, \tag{6b}$$

for $\mu \in (0, 1]$. We note that $f(\mu)$ in Eq. (6a) is the average of the incident particle distribution $F(x, y, \mu, \phi)$ over (x, y) and ϕ.
The major quantities of interest that we intend to compute in this work are the reflection probability

$$R = \frac{\int_0^1 \mu\psi(0, -\mu)\mathrm{d}\mu}{\int_0^1 \mu f(\mu)\mathrm{d}\mu} \tag{7}$$

and the transmission probability

$$T = \frac{\int_0^1 \mu\psi(Z, \mu)\mathrm{d}\mu}{\int_0^1 \mu f(\mu)\mathrm{d}\mu}. \tag{8}$$

At this point, we can use the change of variable [1]

$$\xi = \mu(1 - \mu^2)^{-1/2} \tag{9}$$

to reformulate the problem in a way that will prove to be very convenient for the ADO method. Introducing the dimensionless spatial variable

$$\tau = \frac{L}{\pi A} z, \tag{10}$$

the dimensionless duct length

$$\tau_0 = \frac{L}{\pi A} Z, \tag{11}$$

and the change of notation

$$Y(\tau, \xi) = \psi[\pi A\tau/L, \xi(1 + \xi^2)^{-1/2}] \tag{12}$$

we find that Eq. (5) can be rewritten as

$$\xi\frac{\partial}{\partial\tau} Y(\tau, \xi) + Y(\tau, \xi) = \int_{-\infty}^{\infty} \Psi(\xi')Y(\tau, \xi')\mathrm{d}\xi', \tag{13}$$

for $\tau \in (0, \tau_0)$ and $\xi \in (-\infty, \infty)$. Here, the characteristic function $\Psi(\xi)$ is

$$\Psi(\xi) = \frac{2c}{\pi}(1 + \xi^2)^{-2}. \tag{14}$$

In addition, introducing the change of notation

$$g(\xi) = f[\xi(1+\xi^2)^{-1/2}], \tag{15}$$

we can rewrite the boundary conditions given by Eqs. (6) as

$$Y(0,\xi) = g(\xi) \tag{16a}$$

and

$$Y(\tau_0,-\xi) = 0, \tag{16b}$$

for $\xi \in (0,\infty)$.
Finally, we find that the expressions for the reflection and transmission probabilities given by Eqs. (7) and (8) can be rewritten in terms of ξ-variable integrals as

$$R = \frac{\int_0^\infty \xi(1+\xi^2)^{-2}Y(0,-\xi)\mathrm{d}\xi}{\int_0^\infty \xi(1+\xi^2)^{-2}g(\xi)\mathrm{d}\xi} \tag{17a}$$

and

$$T = \frac{\int_0^\infty \xi(1+\xi^2)^{-2}Y(\tau_0,\xi)\mathrm{d}\xi}{\int_0^\infty \xi(1+\xi^2)^{-2}g(\xi)\mathrm{d}\xi}. \tag{17b}$$

3. THE ADO METHOD

The discrete-ordinates method consists essentially in approximating the integration over the angular variable in the transport equation by a quadrature rule and considering the resulting equation only for the values of the angular variable that coincide with the quadrature nodes. With this procedure, the original integro-differential transport equation is approximated by a system of ordinary differential equations that can be solved in many ways. To avoid the discontinuity in the angular flux that occurs at boundaries and interfaces as the angular variable approaches zero from above and from below, the ADO version of the discrete-ordinates method proposed by Barichello and Siewert [11] makes use of a double quadrature scheme that consists of separate quadrature sets in the positive and negative half-ranges of the angular variable. Using half-range quadrature sets of even order N that are symmetrical about $\xi = 0$ in the ADO method, we obtain the following discrete-ordinates version of Eq. (13) for $i = 1, 2, \ldots, N$:

$$\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} Y(\tau,\xi_i) + Y(\tau,\xi_i) = \sum_{n=1}^{N} w_n \Psi(\xi_n)[Y(\tau,\xi_n) + Y(\tau,-\xi_n)] \tag{18a}$$

and

$$-\xi_i \frac{\mathrm{d}}{\mathrm{d}\tau} Y(\tau,-\xi_i) + Y(\tau,-\xi_i) = \sum_{n=1}^{N} w_n \Psi(\xi_n)[Y(\tau,\xi_n) + Y(\tau,-\xi_n)], \tag{18b}$$

where $\{\xi_n\}$ and $\{w_n\}$ are, respectively, the nodes and weights of our Nth order quadrature rule for integration in $(0,\infty)$ that will be specified later. We note that the discrete-ordinates

equations expressed by Eqs. (18) are formally the same as those encountered when the ADO method is used [12] to solve rarefied gas problems based on the linearized BGK model [13], the only difference being the form of the characteristic function, which is exponential in the case of the BGK model and rational in our case.
As done in previous papers [11, 12], we look for exponential solutions in the form

$$Y(\tau, \pm\xi_i) = \phi(\nu, \pm\xi_i)\mathrm{e}^{-\tau/\nu}, \tag{19}$$

where the parameter ν and the elementary solutions $\phi(\nu, \pm\xi_i)$ are to be determined. As shown by Barichello and Siewert [11], the admissible values of ν (known as *separation constants*) are real and appear in the form of N plus/minus pairs, say $\pm\nu_j$, $j = 1, 2, \ldots, N$. These authors have also shown that the separation constants are related to the eigenvalues of a special $N \times N$ matrix $\boldsymbol{D} - 2\boldsymbol{z}\boldsymbol{z}^T$, where $\boldsymbol{D}$ is a $N \times N$ diagonal matrix and $\boldsymbol{z}$ a column vector of N components that are defined as

$$\boldsymbol{D} = \mathrm{diag}\left\{\xi_1^{-2},\, \xi_2^{-2},\, \ldots,\, \xi_N^{-2}\right\} \tag{20}$$

and

$$\boldsymbol{z} = \begin{pmatrix} \frac{\sqrt{w_1 \Psi(\xi_1)}}{\xi_1} \\ \frac{\sqrt{w_2 \Psi(\xi_2)}}{\xi_2} \\ \vdots \\ \frac{\sqrt{w_N \Psi(\xi_N)}}{\xi_N} \end{pmatrix}, \tag{21}$$

and T denotes the transpose operation. Noting that $\boldsymbol{D} - 2\boldsymbol{z}\boldsymbol{z}^T$ has the structure of a rank-one update of a diagonal matrix, Siewert and Wright [14] developed an efficient algorithm for computing its eigenvalues. Once these eigenvalues, say λ_j, $j = 1, 2, \ldots, N$, are computed, the separation constants are available from

$$\nu_j = \lambda_j^{-1/2}, \tag{22}$$

for $j = 1, 2, \ldots, N$. In addition, assuming that the discrete ordinates $\{\xi_i\}$ are ordered by decreasing magnitudes, we can write the interlacing property mentioned in the work by Siewert and Wright [14] as

$$0 < \xi_N < \nu_N < \xi_{N-1} < \nu_{N-1} < \ldots < \xi_2 < \nu_2 < \xi_1 < \nu_1 \leq \infty, \tag{23}$$

where the equality in the last term holds only if $c = 1$. The interlacing property is important because it shows that a separation constant cannot be equal to an ordinate.
With regard to the elementary solutions, it follows directly from Eqs. (18) that they are given by

$$\phi(\nu_j, \pm\xi_i) = \frac{\nu_j}{\nu_j \mp \xi_i}, \tag{24}$$

for $i, j = 1, 2, \dots, N$, provided the normalization

$$\sum_{n=1}^{N} w_n \Psi(\xi_n)[\phi(\nu_j, \xi_n) + \phi(\nu_j, -\xi_n)] = 1 \tag{25}$$

is used.

Having found the separation constants and the elementary solutions, we now use superposition and write the complete ADO solution to Eqs. (18) for $c < 1$ as

$$Y(\tau, \pm\xi_i) = \sum_{j=1}^{N} [a_j \phi(\nu_j, \pm\xi_i) \mathrm{e}^{-\tau/\nu_j} + b_j \phi(\nu_j, \mp\xi_i) \mathrm{e}^{-(\tau_0-\tau)/\nu_j}], \tag{26}$$

for $i = 1, 2, \dots, N$. As mentioned before, in the event that $c = 1$ one pair of separation constants ($\pm\nu_1$ in our notation) becomes unbounded, and so Eq. (26) needs to be modified. To this end, we follow previous works [15, 16] and replace the elementary solutions that correspond to the unbounded separation constants in Eq. (26) with linear combinations of the exact solutions 1 and $(\tau - \xi)$ of Eq. (13) for $c = 1$, and so we write the complete solution for $c = 1$ as

$$Y(\tau, \pm\xi_i) = a_1(\tau_0 - \tau \pm \xi_i) + b_1(\tau \mp \xi_i) + \sum_{j=2}^{N} [a_j \phi(\nu_j, \pm\xi_i) \mathrm{e}^{-\tau/\nu_j} + b_j \phi(\nu_j, \mp\xi_i) \mathrm{e}^{-(\tau_0-\tau)/\nu_j}], \tag{27}$$

for $i = 1, 2, \dots, N$.

To determine the superposition coefficients $\{a_j\}$ and $\{b_j\}$, we take the ADO solution to satisfy discrete-ordinates versions of the boundary conditions expressed by Eqs. (16). For $c < 1$, we obtain

$$\sum_{j=1}^{N} [a_j \phi(\nu_j, \xi_i) + b_j \phi(\nu_j, -\xi_i) \mathrm{e}^{-\tau_0/\nu_j}] = g(\xi_i) \tag{28a}$$

and

$$\sum_{j=1}^{N} [a_j \phi(\nu_j, -\xi_i) \mathrm{e}^{-\tau_0/\nu_j} + b_j \phi(\nu_j, \xi_i)] = 0, \tag{28b}$$

for $i = 1, 2, \dots, N$. This constitutes a linear system of $2N$ algebraic equations to be solved for $\{a_j\}$ and $\{b_j\}$. Using matrix notation, we rewrite Eqs. (28) as

$$\begin{pmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{B} & \boldsymbol{A} \end{pmatrix} \begin{pmatrix} \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix} = \begin{pmatrix} \boldsymbol{g} \\ \boldsymbol{0} \end{pmatrix}, \tag{29}$$

where

$$\boldsymbol{A} = \begin{pmatrix} \frac{\nu_1}{\nu_1-\xi_1} & \frac{\nu_2}{\nu_2-\xi_1} & \cdots & \frac{\nu_N}{\nu_N-\xi_1} \\ \frac{\nu_1}{\nu_1-\xi_2} & \frac{\nu_2}{\nu_2-\xi_2} & \cdots & \frac{\nu_N}{\nu_N-\xi_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\nu_1}{\nu_1-\xi_N} & \frac{\nu_2}{\nu_2-\xi_N} & \cdots & \frac{\nu_N}{\nu_N-\xi_N} \end{pmatrix}, \tag{30}$$

$$\boldsymbol{B} = \begin{pmatrix} \frac{\nu_1}{\nu_1+\xi_1} & \frac{\nu_2}{\nu_2+\xi_1} & \cdots & \frac{\nu_N}{\nu_N+\xi_1} \\ \frac{\nu_1}{\nu_1+\xi_2} & \frac{\nu_2}{\nu_2+\xi_2} & \cdots & \frac{\nu_N}{\nu_N+\xi_2} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\nu_1}{\nu_1+\xi_N} & \frac{\nu_2}{\nu_2+\xi_N} & \cdots & \frac{\nu_N}{\nu_N+\xi_N} \end{pmatrix} \boldsymbol{E} \tag{31}$$

with

$$\boldsymbol{E} = \mathrm{diag}\{\mathrm{e}^{-\tau_0/\nu_1}, \mathrm{e}^{-\tau_0/\nu_2}, \ldots, \mathrm{e}^{-\tau_0/\nu_N}\}, \tag{32}$$

$$\boldsymbol{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}, \tag{33a}$$

$$\boldsymbol{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}, \tag{33b}$$

and $\mathbf{0}$ denotes a column vector with N zero components. For $c = 1$, we take Eq. (27) to satisfy discrete-ordinates versions of Eqs. (16) to obtain a linear system that can be written as Eq. (29), except that the definitions of the submatrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are changed to

$$\boldsymbol{A} = \begin{pmatrix} \tau_0+\xi_1 & \frac{\nu_2}{\nu_2-\xi_1} & \cdots & \frac{\nu_N}{\nu_N-\xi_1} \\ \tau_0+\xi_2 & \frac{\nu_2}{\nu_2-\xi_2} & \cdots & \frac{\nu_N}{\nu_N-\xi_2} \\ \vdots & \vdots & \ddots & \vdots \\ \tau_0+\xi_N & \frac{\nu_2}{\nu_2-\xi_N} & \cdots & \frac{\nu_N}{\nu_N-\xi_N} \end{pmatrix} \tag{34}$$

and

$$\boldsymbol{B} = \begin{pmatrix} -\xi_1 & \frac{\nu_2}{\nu_2+\xi_1} & \cdots & \frac{\nu_N}{\nu_N+\xi_1} \\ -\xi_2 & \frac{\nu_2}{\nu_2+\xi_2} & \cdots & \frac{\nu_N}{\nu_N+\xi_2} \\ \vdots & \vdots & \ddots & \vdots \\ -\xi_N & \frac{\nu_2}{\nu_2+\xi_N} & \cdots & \frac{\nu_N}{\nu_N+\xi_N} \end{pmatrix} \boldsymbol{E}, \tag{35}$$

with

$$\boldsymbol{E} = \mathrm{diag}\{1, \mathrm{e}^{-\tau_0/\nu_2}, \ldots, \mathrm{e}^{-\tau_0/\nu_N}\}. \tag{36}$$

Finally, we can approximate the integrals in Eqs. (17) with our quadrature scheme to find the following discrete-ordinates approximations to the desired reflection and transmission probabilities:

$$R = \frac{\sum_{i=1}^{N} w_i \xi_i (1+\xi_i^2)^{-2} Y(0,-\xi_i)}{\sum_{i=1}^{N} w_i \xi_i (1+\xi_i^2)^{-2} g(\xi_i)} \tag{37a}$$

and

$$T = \frac{\sum_{i=1}^{N} w_i \xi_i (1+\xi_i^2)^{-2} Y(\tau_0,\xi_i)}{\sum_{i=1}^{N} w_i \xi_i (1+\xi_i^2)^{-2} g(\xi_i)}. \tag{37b}$$

4. COMPUTATIONAL IMPLEMENTATION AND NUMERICAL RESULTS

We begin this section by reporting our choice of quadrature rule for implementing the ADO method. Among several schemes that we tried, the one that worked best is based on mapping the standard Gauss-Legendre quadrature from $[-1, 1]$ into $[0, \infty)$, according to the nonlinear transformation $\xi = (1 + \mu)/(1 - \mu)$ suggested by Gautschi [17]. If $\{\mu_i\}$ and $\{v_i\}$ are, respectively, the nodes and weights of the N-point Gauss-Legendre quadrature, we find that the nodes and weights of our N-point quadrature for integration in $[0, \infty)$ are given, respectively, by

$$\xi_i = \frac{1+\mu_i}{1-\mu_i} \tag{38a}$$

and

$$w_i = \frac{2}{(1-\mu_i)^2} v_i, \tag{38b}$$

for $i = 1, 2, \ldots, N$.

The separation constants $\{\nu_j\}$ were found by using the UPDATER code developed by Siewert and Wright [14] for computing the eigenvalues $\{\lambda_j\}$ of the matrix $\boldsymbol{D} - 2\boldsymbol{z}\boldsymbol{z}^T$, and then Eq. (22), as discussed in Section 3.

The linear system of Eq. (29) was solved using LU decomposition, as implemented in subroutine DGECO from LINPACK [18], and forward elimination followed by back substitution, as implemented in subroutine DGESL, also from LINPACK.

In order to show the merits of the proposed ADO solution, we report in Tables 1–3 our numerical results for the reflection probability R and the transmission probability T of a duct with circular cross section. The particle incidence was taken to be isotropic and uniform by setting $f(\mu) = 1$ in Eq. (6a), and three different values of the ratio between the duct length Z and the duct radius ρ were considered: $Z/\rho = 1.0$, 4.0, and 10.0. Table 1 is for a wall reflection probability c of 0.2, Table 2 for $c = 0.8$, and Table 3 for $c = 1.0$. We note that the numerical results in these tables confirm the physical notion that the reflection and transmission probabilities should increase as the duct wall becomes more reflective. Also, it can be seen that the reflection probability increases and the transmission probability decreases as Z/ρ is increased.

	$Z/\rho = 1.0$		$Z/\rho = 4.0$		$Z/\rho = 10.0$	
N	R	T	R	T	R	T
2	0.0231632	0.364368	0.0246281	0.193672	0.0249692	0.0701287
4	0.0303084	0.518211	0.0366919	0.169903	0.0371332	0.0409655
6	0.0306315	0.528539	0.0375225	0.164472	0.0379337	0.0420983
8	0.0306403	0.529014	0.0375580	0.164143	0.0379672	0.0422384
10	0.0306414	0.529018	0.0375591	0.164133	0.0379683	0.0422473
12	0.0306412	0.529021	0.0375591	0.164132	0.0379682	0.0422478
14	0.0306412	0.529021	0.0375590	0.164132	0.0379682	0.0422478
16	0.0306412	0.529021	0.0375590	0.164132	0.0379682	0.0422478

Table 1. Reflection and transmission probabilities for $c = 0.2$

	$Z/\rho = 1.0$		$Z/\rho = 4.0$		$Z/\rho = 10.0$	
N	R	T	R	T	R	T
2	0.137565	0.443442	0.167393	0.230672	0.173357	0.0905775
4	0.177609	0.642460	0.271520	0.272787	0.286813	0.0753449
6	0.179314	0.654191	0.278276	0.273760	0.293986	0.0758108
8	0.179358	0.654725	0.278564	0.273772	0.294287	0.0758839
10	0.179364	0.654739	0.278574	0.273773	0.294299	0.0758887
12	0.179363	0.654741	0.278575	0.273773	0.294299	0.0758889
14	0.179363	0.654741	0.278575	0.273773	0.294299	0.0758890
16	0.179363	0.654741	0.278575	0.273773	0.294299	0.0758890

Table 2. Reflection and transmission probabilities for $c = 0.8$

It can be verified that the ADO results for the reflection and transmission probabilities reported in Tables 1–3 converge to six correct digits with a half-range quadrature order N between 10 and 14. Considering a degree of precision that is regarded as adequate for practical work, say three digits, we can see that $N = 6$ is sufficient for the ADO method. We have found that this required about 7 μsec of CPU time on a single core of an Intel® Core™ i7-920 processor running at 2.67 GHz. In contrast, a numerical version of the discrete-ordinates method [3] that we have implemented did require 140 μsec of CPU time on the same processor to yield results with three digits of precision for the easiest of the cases studied in Tables 1–3 ($c = 0.2$ and $Z/\rho = 1.0$); for the most difficult case ($c = 1.0$ and $Z/\rho = 10.0$), it required 360 μsec of CPU time.

N	$Z/\rho = 1.0$ R	$Z/\rho = 1.0$ T	$Z/\rho = 4.0$ R	$Z/\rho = 4.0$ T	$Z/\rho = 10.0$ R	$Z/\rho = 10.0$ T
2	0.229537	0.520463	0.386657	0.363343	0.497593	0.252407
4	0.265404	0.720756	0.534771	0.451388	0.711442	0.274717
6	0.266985	0.732420	0.543497	0.455908	0.723868	0.275537
8	0.267024	0.732953	0.543874	0.456103	0.724402	0.275575
10	0.267029	0.732970	0.543889	0.456110	0.724423	0.275576
12	0.267029	0.732971	0.543889	0.456111	0.724423	0.275576
14	0.267029	0.732971	0.543889	0.456111	0.724424	0.275576
16	0.267029	0.732971	0.543889	0.456111	0.724424	0.275576

Table 3. Reflection and transmission probabilities for $c = 1.0$

5. CONCLUSIONS

We have developed in this work what we believe to be an accurate and efficient discrete-ordinates solution to the Prinja-Pomraning model of neutral particle transport in ducts. For three-digit precision, our method has been found to be between 20 and 50 times faster than a purely numerical version of the discrete-ordinates method. Such a good performance is a motivation for our continuing work on the ADO method for higher-order models [3, 4] of particle transport in ducts.

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