Annals of Nuclear Energy xxx (2013) xxx–xxx

Contents lists available at SciVerse ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

The line source problem in anisotropic neutron transport with internal reflection

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ARTICLE INFO

Article history:
Received 28 November 2012
Received in revised form 7 May 2013
Accepted 9 May 2013
Available online xxxx

Keywords:
Radiative transfer
Spherical harmonics method
Green's function
Integral transforms

ABSTRACT

The three-dimensional radiative transport equation is solved for modeling the propagation of neutrons due to a line source which is placed in an anisotropically scattering half-space medium considering the effect of internal reflection at the interface. The application of the Fourier transform in the transverse directions and a modified spherical harmonics transform with respect to the angular variables lead to an expression for the specific intensity in terms of analytical functions. The final results are verified with Monte Carlo simulations.

1. Introduction

One of the classic problems in multi-dimensional neutron transport theory which is closely related to the searchlight problem (Siewert and Dunn, 1989) is that of a line source which is placed within a scattering half-space medium (Williams, 1982; Loyalka and Williams, 2009). The motion and interaction of neutrons with materials are described with the neutron transport equation (RTE) (Case and Zweifel, 1967; Duderstadt and Martin, 1979). Besides the reactor physics field, line sources are also involved in different applications of nuclear medicine or in the radiative heat transfer (Carslaw and Jaeger, 1959). The line source problem in the half-space geometry with an internal reflecting surface has been solved analytically by Williams (1982) and Williams (2007). The obtained solutions are based on a line source which is placed perpendicular to the surface of an isotropically scattering medium. The theory is developed by considering different integral transforms together with the Wiener–Hopf technique and making use of the generalized Chandrasekhar *H*-functions (Williams, 2007). In addition, the solution of the corresponding diffusion equation (DE) is presented and compared to the transport theory with satisfactory agreements (Williams, 2007). In the publication of Loyalka and Williams (2009) the authors make use of the analytical solutions obtained in Williams (2007) and report numerous numerical results which are useful for verification. In the case of anisotropic scattering solutions to the multi-dimensional RTE are mainly based on numerical methods or approximative equations. The Monte Carlo (MC) method was frequently used as numerical solution of the RTE (Duderstadt and Martin, 1979), but also other techniques like the finite element (Mohan et al., 2011), the finite-difference (Hielscher et al., 1998) or the discrete-ordinate method (Ganapol, 2011) were applied.

In this article we consider the line source problem for the case of an anisotropic scattering half-space medium with internal reflection. To this end we start in the same way as Williams by performing a two-dimensional Fourier transform with respect to the transverse directions. Then, the infinite medium line spread function is derived by making use of the modified spherical harmonics (SH) method (Markel, 2004; Panasyuk et al., 2006; Machida et al., 2010). Finally, the boundary-value problem in the semi-infinite geometry is solved via superposition of the homogeneous and particular solution. The obtained equations are compared with the Monte Carlo method and with the diffusion approximation (DA).

2. Theory

The specific intensity $I(\mathbf{r}, \hat{\mathbf{s}})$ caused by the internal source $S(\mathbf{r}, \hat{\mathbf{s}})$ obeys the three-dimensional RTE (Williams, 2007)

$$\hat{\mathbf{s}} \cdot \nabla I(\mathbf{r}, \hat{\mathbf{s}}) + \mu_t I(\mathbf{r}, \hat{\mathbf{s}}) = \mu_s \int I(\mathbf{r}, \hat{\mathbf{s}}') f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}') \, d^2 s' + S(\mathbf{r}, \hat{\mathbf{s}}), \tag{1}$$

where $\mu_t = \mu_a + \mu_s$ is the total attenuation coefficient, μ_a the absorption coefficient and μ_s the scattering coefficient. The unit vector $\hat{\mathbf{s}} = (\mu, \phi)$ with $\mu = \cos\theta$ specifies the direction of the particle propagation and $f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')$ is the probability density function for describing the direction of the scattered neutrons. In order to solve

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0306-4549/$ - see front matter © 2013 Published by Elsevier Ltd.
http://dx.doi.org/10.1016/j.anucene.2013.05.007

Eq. (1) subject to boundary conditions we afore consider the interactions of neutrons far from interfaces which leads to the solution for the infinite medium. After that the boundary-value problem is solved via superposition of the homogeneous and particular solution.

2.1. Green's function for the infinite medium

In this section Eq. (1) is considered for an infinitely long isotropic line source $S(\mathbf{r},\hat{\mathbf{s}}) = \delta(x)\delta(y)/(4\pi)$ in a three-dimensional uniform medium. Due to the given cylinder symmetry the expected solution will be independent on the spatial variable z. By expanding the specific intensity in form of the Fourier integral

$$I(\mathbf{r},\hat{\mathbf{s}}) = \frac{1}{(2\pi)^2}\int I(\mathbf{q},z,\hat{\mathbf{s}})e^{i\mathbf{q}\cdot\boldsymbol{\rho}}\,\mathrm{d}^2q \tag{2}$$

Eq. (1) becomes in the two-dimensional spatial frequency domain

$$[\mu_t + iq\sin\theta\cos(\phi-\phi_{\mathbf{q}})]I(\mathbf{q},\hat{\mathbf{s}}) = \mu_s\int I(\mathbf{q},\hat{\mathbf{s}}')f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\,\mathrm{d}^2s' + \frac{1}{4\pi}. \tag{3}$$

In order to solve the above integral equation the specific intensity is expanded in terms of spherical harmonics (SH)

$$I(\mathbf{q},\hat{\mathbf{s}}) = \sum_{l=0}^{\infty}\sum_{M=-l}^{l} I_{lM}(q)Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}), \tag{4}$$

whose orientation coincides with the direction of the unit vector $\hat{\mathbf{k}} = (\cos\phi_{\mathbf{q}},\sin\phi_{\mathbf{q}},0)$. Thus, $\hat{\mathbf{k}}$ represents the two-dimensional wave vector $\hat{\mathbf{q}}$. The rotated SH $Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})$ are given by a linear combination of $2l+1$ conventional spherical functions $Y_{lm}(\hat{\mathbf{s}}) = Y_{lm}(\hat{\mathbf{s}};\hat{\mathbf{z}})$ (Panasyuk et al., 2006; Machida et al., 2010)

$$Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \sum_{m=-l}^{l} d^l_{mM}(\theta_{\mathbf{k}})Y_{lm}(\hat{\mathbf{s}})e^{-im\phi_{\mathbf{k}}}, \tag{5}$$

where $d^l_{mM}(\theta_{\mathbf{k}})$ is the Wigner d-function. In the following the angles of rotation are given by $\theta_{\mathbf{k}} = \pi/2$ and $\phi_{\mathbf{k}} = \phi_{\mathbf{q}}$. In that case the Wigner d-function takes the value

$$d^l_{m0}(\pi/2) = \frac{2^m}{\sqrt{\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}\cos\left(\frac{l+m}{2}\pi\right)\frac{\Gamma[(l+m+1)/2]}{\Gamma[(l-m+2)/2]}, \tag{6}$$

where $\Gamma(x)$ denotes the Gamma function. The rotationally invariant scattering phase function depends only on the cosine $\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}'$ and becomes in SH decomposition the form

$$f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}') = \sum_{lM} f_l Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})Y^*_{lM}(\hat{\mathbf{s}}';\hat{\mathbf{k}}), \tag{7}$$

where f_l are the expansion coefficients which are given by

$$f_l = 2\pi\int_{-1}^{1} f(\mu)P_l(\mu)\,\mathrm{d}\mu. \tag{8}$$

Due to reasons regarding the numerical implementation all SH series are truncated at $l_{\max} = N$, where $I_{-1,M}(q) = I_{N+1,M}(q) = 0$ and N is always assumed to be an odd number. Now by inserting (4) in (3), making use of the recurrence relation

$$(\hat{\mathbf{k}}\cdot\hat{\mathbf{s}})Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}}) = \sqrt{\frac{l^2-M^2}{4l^2-1}}Y_{l-1,M}(\hat{\mathbf{s}};\hat{\mathbf{k}}) + \sqrt{\frac{(l+1)^2-M^2}{4(l+1)^2-1}}Y_{l+1,M}(\hat{\mathbf{s}};\hat{\mathbf{k}}), \tag{9}$$

as well as the orthogonality

$$\int Y_{lM}(\hat{\mathbf{s}};\hat{\mathbf{k}})Y^*_{l',M'}(\hat{\mathbf{s}};\hat{\mathbf{k}})\,\mathrm{d}^2s = \delta_{ll'}\delta_{MM'}, \tag{10}$$

we obtain the following set of linear equations

$$iq\sqrt{\frac{l^2-M^2}{4l^2-1}}I_{l-1,M}(q) + iq\sqrt{\frac{(l+1)^2-M^2}{4(l+1)^2-1}}I_{l+1,M}(q) + \sigma_l I_{lM}(q) = \frac{\delta_{l0}\delta_{M0}}{\sqrt{4\pi}}, \tag{11}$$

where $\sigma_l = \mu_a + (1-f_l)\mu_s$ and $l = 0,\ldots,N$. The above system has in principle the same relatively simple structure as the P_N equations for plane symmetric radiative transfer problems (Case and Zweifel, 1967) which is due to the rotated reference frame. Note also that a result of the isotropic line source is that we only must consider one system namely for the value $M = 0$ resulting in $N+1$ linear equations. On the other hand more complicated sources such as the unidirectional line source can be directly implemented by calculating the corresponding expansion coefficients. In matrix notation system (11) can be written as $(T^2 + iq\,W)|I\rangle = |b\rangle$, with vector components $\langle l|I\rangle = I_{l0}(q)$ and $\langle l|b\rangle = \delta_{l0}/\sqrt{4\pi}$. The matrix T is a diagonal matrix with elements $T_{ll'} = \sqrt{\sigma_l}\delta_{ll'}$. Next, we consider the symmetric tridiagonal matrix

$$T^{-1}WT^{-1} = \begin{pmatrix} 0 & \beta_1 & 0 & 0 & \cdots & 0 \\ \beta_1 & 0 & \beta_2 & 0 & \cdots & \vdots \\ 0 & \beta_2 & \ddots & \ddots & \cdots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \cdots & \cdots & \ddots & 0 & \beta_N \\ 0 & \cdots & 0 & 0 & \beta_N & 0 \end{pmatrix}, \tag{12}$$

where $\beta_l = l/\sqrt{(2l-1)(2l+1)\sigma_{l-1}\sigma_l}$. By performing uniquely the eigenvalue decomposition (EVD) $U\Lambda U^{-1} = T^{-1}WT^{-1}$, the solution of (11) can be obtained with an analytical dependence on the scalar wave number q. The EVD yields all in all $N+1$ real-valued eigenvalues λ_i which appear in pairs. An eigenvalue λ_i corresponds with an eigenvector $|v_i\rangle$ having components $\langle l|v_i\rangle$, whereas the negative value $-\lambda_i$ leads to the components $(-1)^l\langle l|v_i\rangle$ (Markel, 2004). After some algebraic rearrangement we find

$$I_{lM}(q) = \frac{\delta_{M0}}{2\sqrt{\pi\sigma_0\sigma_l}}\sum_{\lambda_i}\frac{\langle l|v_i\rangle\langle v_i|0\rangle}{1+iq\lambda_i}. \tag{13}$$

By inserting (13) in (4) and considering the above mentioned properties of the eigenvector components we arrive at the line spread function in Fourier space

$$I(\mathbf{q},z,\hat{\mathbf{s}}) = \sum_{l=0}^{N}\sum_{m=-l}^{l} I_{lm}(q)Y_{lm}(\hat{\mathbf{s}})e^{-im\phi_{\mathbf{q}}}, \tag{14}$$

with coefficients

$$I_{lm}(q) = \frac{1}{2\sqrt{\pi\sigma_0\sigma_l}}\sum_{\lambda_i>0}\frac{\langle l|v_i\rangle\langle v_i|0\rangle}{\lambda_i^2} \times \frac{1+(-1)^l - iq\lambda_i[1-(-1)^l]}{q^2+1/\lambda_i^2}d^l_{m0}(\pi/2). \tag{15}$$

The inverse Fourier transform regarding the angular variable can be performed by making use of the relation

$$\int_0^{2\pi} e^{iq\rho\cos(\phi_{\mathbf{q}}-\phi_\rho)}e^{-im\phi_{\mathbf{q}}}\,\mathrm{d}\phi_{\mathbf{q}} = 2\pi i^m J_m(q\rho)e^{-im\phi_\rho}, \tag{16}$$

where $J_m(x)$ is the Bessel function of the first kind. Note that the value $d^l_{m0}(\pi/2)$ is only non-zero if $l+m$ is even which leads to the fact that the sign of $(-1)^l$ from (15) coincides with that of $(-1)^m$. Thus, the resulting inverse Hankel transform becomes exactly the same as for the two-dimensional infinitely extended disc geometry (Liemert and Kienle, 2011). Upon its evaluation the specific

Please cite this article in press as: Liemert, A., Kienle, A. The line source problem in anisotropic neutron transport with internal reflection. Ann. Nucl. Energy (2013), http://dx.doi.org/10.1016/j.anucene.2013.05.007

intensity for the unbounded anisotropically scattering medium is obtained as

$$I(\boldsymbol{\rho},\hat{\mathbf{s}}) = \sum_{l=0}^{N}\sum_{m=-l}^{l} I_{lm}(\rho)Y_{lm}(\theta,\chi), \tag{17}$$

where $\chi = \phi - \phi_{\boldsymbol{\rho}}$. The corresponding expansion coefficients become

$$I_{lm}(\rho) = \frac{d^l_{m0}(\pi/2)}{2\pi\sqrt{\pi\sigma_0\sigma_l}}\sum_{\lambda_i>0}\frac{\langle l|v_i\rangle\langle v_i|0\rangle}{\lambda_i^2}K_m(\rho/\lambda_i), \tag{18}$$

where $K_m(x)$ is the modified Bessel function of the second kind. The fluence $\Phi(\rho)$ and the current $\mathbf{J}(\boldsymbol{\rho})$ for the infinite medium are obtained via integration of the specific intensity resulting in

$$\Phi(\rho) = \int I(\mathbf{r},\hat{\mathbf{s}})\ \mathrm{d}^2s = \frac{1}{\pi\sigma_0}\sum_{\lambda_i>0}\frac{\langle 0|v_i\rangle\langle v_i|0\rangle}{\lambda_i^2}K_0(\rho/\lambda_i), \tag{19}$$

$$\mathbf{J}(\boldsymbol{\rho}) = \int \hat{\mathbf{s}}I(\mathbf{r},\hat{\mathbf{s}})\ \mathrm{d}^2s = \frac{\hat{\boldsymbol{\rho}}}{\pi}\sum_{\lambda_i>0}\frac{\langle 0|v_i\rangle\langle v_i|0\rangle}{\lambda_i}K_1(\rho/\lambda_i). \tag{20}$$

2.2. The line source problem in the semi-infinite geometry

In this section the derived Green's function for the infinite medium is used for solving the line source problem in the semi-infinite geometry. The exact BC for obtaining the semi-infinite geometry is defined in $\hat{\mathbf{s}}\cdot\hat{\mathbf{z}} > 0$ and given by

$$I(\rho, z=0,\mu,\phi) = R(\mu)I(\rho, z=0,-\mu,\phi), \tag{21}$$

where $R(\mu)$ is Fresnel reflection coefficient (Williams, 2005). In order to satisfy the above BC we additionally must provide the general solution to the homogeneous RTE in the spatial frequency domain

$$\begin{aligned}&[\cos\theta\partial_z + iq\sin\theta\cos(\phi-\phi_{\mathbf{q}}) + \mu_t]I(\mathbf{q},z,\hat{\mathbf{s}})\\ &\quad = \mu_s\int I(\mathbf{q},z,\hat{\mathbf{s}}')f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')\ \mathrm{d}^2s',\end{aligned} \tag{22}$$

where $I(\mathbf{q},z,\hat{\mathbf{s}}) \to 0$ for $z\to\infty$. Next, we seek solutions in form of the plane wave mode

$$I(\mathbf{q},z,\hat{\mathbf{s}}) = \exp(-\xi z)\sum_{lm}\psi_{lm}(q)Y_{lm}(\hat{\mathbf{s}})\exp(-im\phi_{\mathbf{q}}), \tag{23}$$

where the orientation of the SH coincides again with the direction of the transverse wave vector $\mathbf{q}$. Therefore we obtain the following eigenvalue problem parameterised by $l = m,\ m+1,\ldots,N$ for $m = 0,1,\ldots,N$ according to

$$\begin{aligned}&-\xi\left[\frac{a_{lm}}{\sqrt{2l-1}}\psi_{l-1,m}(q) + \frac{a_{l+1,m}}{\sqrt{2l+3}}\psi_{l+1,m}(q)\right]\\ &+iq[b_{l-1,m}\psi_{l-1,m+1}(q) - c_{l+1,m}\psi_{l+1,m+1}(q)]\\ &+iq[b_{l+1,m}\psi_{l+1,m-1}(q) - c_{l-1,m}\psi_{l-1,m-1}(q)]\\ &+\sqrt{2l+1}\sigma_l I_{lm}(q) = 0,\end{aligned} \tag{24}$$

with the quantities $\sigma_l = \mu_a + (1-f_l)\mu_s$. The number of linear equations is $(N+1)(N+2)/2$. Furthermore we have $a_{lm} = \sqrt{l^2-m^2}$, $b_{lm} = c_{l,-m}$ and $c_{lm} = \sqrt{(l+m)(l+m+1)/(2l+1)}/2$. In matrix notation the eigenvalue problem can be written as $(S+iqB)|u(q)\rangle = \xi A|\ u(q)\rangle$, where the eigenvector components are given by $\langle n|u(q)\rangle$ for $1\leqslant n\leqslant (N+1)(N+2)/2$. The corresponding characteristic equation is

$$\prod_{\lambda_i>0}(1-\xi^2\lambda_i^2) = 0, \tag{25}$$

where λ_i are the eigenvalues of the matrix $(S+iqB)^{-1}A$. The corresponding nontrivial solution $|u_i(q)\rangle \neq \mathbf{0}$ to the eigenvalue $\xi_i = 1/\lambda_i$ is given by the eigenvector of $B^{-1}A$ to the value λ_i. The expansion coefficients and the eigenvector components are related by

$$\psi_{lm}(q) = \langle l+1+mN - m(m-1)/2|u(q)\rangle. \tag{26}$$

The homogeneous solution for the semi-infinite geometry is now obtained as

$$I^{(h)}(\mathbf{r},\hat{\mathbf{s}}) = \sum_{lm}\psi_{lm}(\rho,z)Y_{lm}(\theta,\chi), \tag{27}$$

where

$$\psi_{lm}(\rho,z) = \frac{i^m}{2\pi}\int_0^\infty \psi_{lm}(q,z)J_m(q\rho)q\ \mathrm{d}q, \tag{28}$$

with

$$\psi_{lm}(q,z) = \sum_{\xi_i>0}C_i(q)\exp(-\xi_i z)\psi^{(i)}_{lm}(q). \tag{29}$$

The general solution to the RTE (1) is now obtained via superposition of the homogenous and particular part. In order to determine the unknown constants the BC (21) is formulated according to Marshak's method (Modest, 2003)

$$\int_{\mu>0} I(\rho,z=0,\mu,\phi)Y^*_{l'm'}(\hat{\mathbf{s}})\,\mathrm{d}^2s = \int_{\mu>0} R(\mu)I(\rho,z=0,-\mu,\phi)Y^*_{l'm'}(\hat{\mathbf{s}})\,\mathrm{d}^2s, \tag{30}$$

so that we can generate a system of $(N+1)^2/4$ linear equation for finding the unknown constants $C_i(q)$.

3. Verification

In this section the derived transport theory solutions are verified and illustrated by comparisons with the MC method (Kienle and Hibst, 2006) and the DA, respectively. The corresponding solution of the diffusion equation for the line source problem can be found in Williams (2007). We refer to the developed analytical method for solving the RTE in the following as the spherical harmonics method (SHM). For modeling the interactions of neutrons within an anisotropically scattering medium we apply as an example the Henyey–Greenstein model as probability density function which has the explicit form

$$f(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}') = \frac{1}{4\pi}\frac{1-g^2}{[1+g^2-2g(\hat{\mathbf{s}}\cdot\hat{\mathbf{s}}')]^{3/2}}, \tag{31}$$

whereas in terms of rotated SH according to (4) this function is given exactly for the coefficients $f_l = g^l$. The refractive index of the surrounding medium is assumed to be $n_0 = 1.0$ in all simulations. The occurrent integrals are evaluated by using the Gaussian Legendre quadrature method.

We start the comparisons with the fluence in the infinitely extended anisotropically scattering medium. Fig. 1 displays the fluence versus radial distance to the isotropic line source computed with Eq. (19) (solid line), the MC method (filled dots) and the DA (dashed line). The inset shows the relative differences to the MC method which have been calculated for both the SHM and the DA. It can be seen that the DA shows significant differences to the MC simulation in contrast to the SHM.

Fig. 2 shows the fluence at the depth $z = 1$ mm in the semi-infinite medium as function of the radial distance caused by a isotropic line source. The result obtained from the derived solution corresponds with the solid line whereas the filled dots display the MC method. Again, we computed the relative differences between the MC method, the SHM and the DA which can be seen in the inset of Fig. 2. Similar as in Fig. 1 the DE shows systematic differences compared to the MC especially at small distances to the source. The relative differences between the SHM and the MC simulations

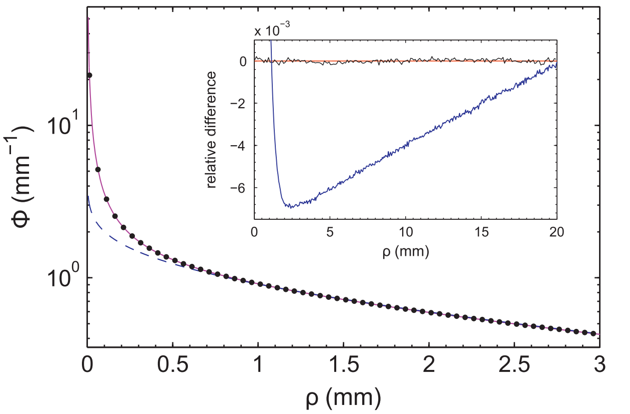

Fig. 1. Internal fluence versus radial distance due to a isotropic line source in an infinitely extended anisotropically scattering medium. The properties of the infinite medium are $\mu_a = 0.01\ \text{mm}^{-1}$, $\mu_s = 5\ \text{mm}^{-1}$ and $g = 0.8$.

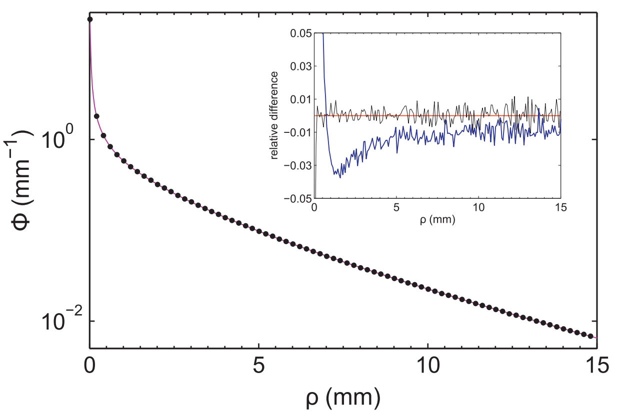

Fig. 2. Internal fluence versus radial distance in the semi-infinite medium due to a isotropic line source which is perpendicular to the boundary. The anisotropically scattering half-space is characterized by the parameters $\mu_a = 0.01\ \text{mm}^{-1}$, $\mu_s = 2.5\ \text{mm}^{-1}$, $g = 0.6$ and $n = 1.4$.

can be further reduced by increasing the number of simulated particles.

4. Conclusions and discussion

In this article we derived an analytical framework for accurate modeling the transport of neutrons within an anisotropically scattering semi-infinite medium including the effect of internal reflection. To this end the line source problem was solved by making use of integral transforms as well as under consideration of results from our earlier publication. In the results section the Henyey–Greenstein function was applied as scattering function, but the derived equations can be used for an arbitrary rotationally invariant scattering phase function.

The obtained equations were successfully verified and illustrated with comparisons to the MC method and the DA for the case of the isotropic line source. However the general theory is expandable to more complicated source types such as the exponential decaying line source having the same angular distribution as the applied scattering phase function $f(\hat{\mathbf{s}} \cdot \hat{\mathbf{s}}')$. Besides the direct application of the derived equations for solving different line source problems in radiative transfer it can also be used for validation of standard commercial reactor physics computer codes or to estimate the accuracy of the applied approximation order within the conventional spherical harmonics method.

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