Annals of Nuclear Energy 65 (2014) 376–384

Contents lists available at ScienceDirect

Annals of Nuclear Energy

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

Spherical shields perturbed to ellipsoids in transport theory

Jeffrey A. Favorite *

Monte Carlo Methods, Codes, and Applications (XCP-3), MS F663, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

ARTICLE INFO

Article history:
Received 21 August 2013
Received in revised form 6 November 2013
Accepted 7 November 2013
Available online 13 December 2013

Keywords:
Perturbation theory
Surface perturbation theory
Gamma rays

ABSTRACT

One-dimensional spheres are perturbed to ellipsoids, and perturbation theory for inhomogeneous transport problems is applied to estimate the leakage of an uncollided decay gamma ray, a neutron thermal capture gamma ray, and a neutron inelastic scatter gamma ray. Only the shielding is perturbed, not the source. The surface transformation function for the sphere-to-ellipsoid change-of-shape perturbation is derived. Schwinger, Roussopolos, and combined perturbation estimates are applied. The perturbation estimates are defined to estimate the total (4π) flux at an external spherical surface detector, and they were accurate for point-detector fluxes when the leakage estimated from a point detector was similar to the total external surface flux. For uncollided line fluxes, the Schwinger estimate worked very well when the response of interest was the total external surface flux, but perturbation theory did not work well when the response of interest was the flux measured at a single external point (unless extra care was taken to account for geometric effects). For thermal capture line fluxes, the Roussopolos estimate was extremely accurate for one point detector location but its accuracy depended on the detector location. For inelastic scatter line fluxes, the detector fluxes were relatively insensitive to the detector location and the perturbation estimates were fairly accurate.

1. Introduction

Because of the speed, low memory requirement, and overall simplicity of one-dimensional calculations, it is often desirable to solve radiation transport problems in one-dimensional spherical geometries even if the actual object being modeled is not spherical. Recently, we proposed treating nonspherical geometries as perturbations of spherical geometries using surface perturbation theory for the inhomogenous Boltzmann transport equation (Favorite, 2013). In test problems involving uncollided decay gamma rays and neutron-induced gamma rays, spherical shields were perturbed to nonspherical shields: a radial expansion or contraction within a 45-degree cone and a more extreme change of shape to a cube. The response of interest was the gamma-ray flux measured at an external detector.

In this paper, we apply perturbation theory to the change of shape from a sphere to an ellipsoid. As in Favorite (2013), the surface perturbation methods developed by Rahnema (1984, 1996) are applied with the Schwinger (Bell and Glasstone, 1970; Stacey, 1974, 2001) and Roussopolos (Stacey, 1974, 2001) variational functionals. The unperturbed test problem geometry and materials are the same as those used in Favorite (2013). As in Favorite (2013), only the shielding is perturbed, not the source, and we present results involving uncollided photons as well as coupled neutron-gamma-ray fields with scattering.

As in Favorite (2013), the calculations were done with a one-dimensional ray-tracing code (Favorite et al., 2009), with the continuous-angle Monte Carlo code MCNP6 (Pelowitz, 2013), with MCNP6 modified with a special-purpose uncollided flux patch (Favorite, 2012), and with the multigroup discrete ordinates code PARTISN (Alcouffe et al., 2008).

The next section of this paper presents only enough background material to establish the notation. Section 3 briefly discusses the geometries, materials, and methods that were used in the calculations. Details missing from Section 2 and 3 may be found in Favorite (2013). Section 4 presents the results for the sphere-to-ellipsoid transformation, including the derivation of the surface transformation function. Section 5 is a summary.

2. Perturbation theory

Consider a system that includes some volumetric source of neutral particles surrounded by some shield. Both the source and the shield may be multilayered but, for simplicity, only homogeneous layers are considered. The Boltzmann transport equation, rendered in operator notation as

$$L\psi = q, \tag{1}$$

can be solved for this system to give $\psi(\vec{\mathbf{r}}, E, \widehat{\boldsymbol{\Omega}})$, the angular flux of particles of energy E, position $\vec{\mathbf{r}}$, and direction $\widehat{\boldsymbol{\Omega}}$. In Eq. (1), L is the transport operator and q is the particle source density. Suppose a set of D measurements is taken at a detector or set of detectors. These may be, for example, peaks in a gamma-ray spectrum from

* Tel.: +1 505 667 7941; fax: +1 505 665 2879.
E-mail address: fave@lanl.gov

0306-4549/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.anucene.2013.11.011

which the flux or leakage of gamma-ray lines is obtained. The quantities of interest are

$$M_d = \langle \Sigma_d \psi \rangle, \; d = 1, \ldots, D, \tag{2}$$

where the detector response function $\Sigma_d(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}})$ is defined as zero outside the detector volume, angle, and energy region of interest to detector d. A weight function or energy- or angle-dependent detector efficiency can be built into $\Sigma_d(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}})$. In this paper, as in Favorite (2013), M_d will be either the flux integrated over a spherical 4π detector located a distance $r_{d,4\pi}$ from the origin or the flux at a point $\vec{\mathbf{r}}_d$ multiplied by the surface area of an assumed spherical 4π detector intersecting $\vec{\mathbf{r}}_d$. The equation for the adjoint flux $\psi^*(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}})$, again in operator notation, is

$$L^* \psi^* = \Sigma_d. \tag{3}$$

Now suppose the system is perturbed in some way. If the detector and the external boundaries and boundary conditions are not perturbed, the exact value of the perturbed response of interest for detector d is

$$M'_d = \langle \Sigma_d \psi' \rangle = \langle \Sigma_d (\psi + \Delta\psi) \rangle \tag{4}$$

where a prime indicates a perturbed quantity and a Δ indicates the perturbation.

A variational functional for M'_d is the Schwinger functional (Bell and Glasstone, 1970; Stacey, 1974, 2001), which can be written as (Favorite, 2006, 2007)

$$M_{d,S}[\psi^*, \psi] = \langle \Sigma_d \psi \rangle \frac{\langle \psi^* q \rangle + \langle \psi^* \Delta q \rangle}{\langle \psi^* q \rangle + \langle \psi^* \Delta L \psi \rangle}. \tag{5}$$

Another variational functional for M'_d is the Roussopolos functional (Stacey, 1974, 2001), which can be written as (Favorite, 2006, 2007)

$$M_{d,R}[\psi^*, \psi] = \langle \Sigma_d \psi \rangle - \langle \psi^* (\Delta L \psi - \Delta q) \rangle. \tag{6}$$

A combined Schwinger–Roussopolos functional for M'_d was presented in Favorite (2006) and written as

$$M_{d,C}[f, \psi^*, \psi] = \langle \Sigma_d \psi \rangle \frac{\langle \psi^* q \rangle + \langle f \psi^* \Delta q \rangle}{\langle \psi^* q \rangle + \langle f \psi^* \Delta L \psi \rangle} - \langle (1-f) \psi^* (\Delta L \psi - \Delta q) \rangle, \tag{7}$$

where f is a factor to be determined. Using $f = 0$ yields the Roussopolos functional, $f = 1$ yields the Schwinger functional, and $0 < f < 1$ yields some combination. In spherical problems when the source was not perturbed, $f = 1/\sqrt{2}$ yielded excellent results for the uncollided decay gamma-ray leakage (Favorite, 2006, 2013).

The inner products of perturbed quantities in Eqs. (5)–(7) contain volume integrals that are nonzero only in the region between the unperturbed and the perturbed interfaces. As in Favorite (2013), we apply the "surface-layer formula" (Rahnema, 1996)

$$\int_{\Delta V} dV(\cdot) \approx \int_{S(V)} dSX(\cdot), \tag{8}$$

where ΔV is the perturbed volume, $S(V)$ is the boundary of the unperturbed volume (i.e., the unperturbed surface), and X is the *surface transformation function*, or the distance between the perturbed and unperturbed surfaces in the direction of the outward normal of the unperturbed surface. To be specific, the inner products in question become

$$\begin{aligned} \langle \psi^* \Delta L \psi \rangle &= \int_{\Delta V} dV \int_{4\pi} d\widehat{\mathbf{\Omega}} \int_0^\infty dE \psi^*(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}}) [\Delta L(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}}) \psi(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}})] \\ &\approx \int_{S_0} dSX(\vec{\mathbf{r}}_n) \int_{4\pi} d\widehat{\mathbf{\Omega}} \int_0^\infty dE \psi^*(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) [\Delta L(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \psi(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}})] \end{aligned} \tag{9}$$

and

$$\begin{aligned} \langle \psi^* \Delta q \rangle &= \int_{\Delta V} dV \int_{4\pi} d\widehat{\mathbf{\Omega}} \int_0^\infty dE \psi^*(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}}) \Delta q(\vec{\mathbf{r}}, E, \widehat{\mathbf{\Omega}}) \\ &\approx \int_{S_0} dSX(\vec{\mathbf{r}}_n) \int_{4\pi} d\widehat{\mathbf{\Omega}} \int_0^\infty dE \psi^*(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \Delta q(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}), \end{aligned} \tag{10}$$

where $\vec{\mathbf{r}}_n$ represents the points on the unperturbed surface S_0 and $\Delta A(\vec{\mathbf{r}}_n)$ means the value of A on the negative side of surface S_0 minus the value on the positive side.

Because the unperturbed geometries in this paper are one-dimensional spheres, the angle and energy integrals of the fluxes in Eqs. (9) and (10) are constants that may be removed from the surface integral. Eqs. (9) and (10) become

$$\langle \psi^* \Delta L \psi \rangle \approx \frac{\int_{S_0} dSX(\vec{\mathbf{r}}_n)}{4\pi r_n^2} \left\{ (4\pi r_n^2) \int_{4\pi} d\widehat{\mathbf{\Omega}} \int_0^\infty dE \psi^*(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \left[\Delta L(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \psi(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \right] \right\} \tag{11}$$

and

$$\langle \psi^* \Delta q \rangle \approx \frac{\int_{S_0} dSX(\vec{\mathbf{r}}_n)}{4\pi r_n^2} \left\{ (4\pi r_n^2) \int_{4\pi} d\widehat{\mathbf{\Omega}} \int_0^\infty dE \psi^*(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \Delta q(\vec{\mathbf{r}}_n, E, \widehat{\mathbf{\Omega}}) \right\}, \tag{12}$$

where $r_n = \|\vec{\mathbf{r}}_n\|$. The area of the unperturbed surface, $4\pi r_n^2$, appears because the quantity in braces in Eq. (11) was computed in Favorite (2013). In this paper, as in Favorite (2013), there are no source perturbations, so Eqs. (10) and (12) are not used.

For more details, see Favorite (2013).

3. Geometry, materials, and methods

The computational test objects used three materials: high-enriched uranium (HEU), stainless steel (SS) 304, and a material containing carbon, hydrogen, nitrogen, and oxygen (CHNO). The density and composition of these materials are given in Table 1. For the HEU density and composition given in Table 1, the source rate q of the 766-keV line from decay of ^{238}U is 38.09993 γ/cm^3 s (Gunnick and Tinney, 1971). The macroscopic photon cross sections Σ_t for the HEU and SS at 766 keV are given in Table 2 (White, 2003). These cross sections do not include coherent scattering. Two of the neutron-induced gamma-ray lines produced in the CHNO material are shown with their production mechanisms in Table 3.

The problem with uncollided decay photons used an initial, unperturbed geometry having a 10-kg sphere of HEU (radius of 5.03169067346416 cm) for the source. It had the source encased tightly (no gaps) in a shell of SS with an outer radius of 7 cm. In this paper, the outer surface of the SS is perturbed to an ellipsoid. Only the 766-keV uranium line was used. The uncollided line flux "measured" at an external detector located at point $\vec{\mathbf{r}}_d$ was computed using a one-dimensional spherical ray-tracing code (Favorite

Table 1
Material specifications.

Material	Density (g/cm^3)	Isotope	Wgt. fraction
HEU	18.74	^{235}U	0.9473
		^{238}U	0.0527
SS 304	7.86	^{50}Cr	0.008278
		^{52}Cr	0.159452
		^{53}Cr	0.018078
		^{54}Cr	0.004491
		^{55}Mn	0.020000
		^{54}Fe	0.040944
		^{56}Fe	0.642158
		^{57}Fe	0.014838
		^{58}Fe	0.001960
		^{58}Ni	0.061136
		^{60}Ni	0.023546
		^{61}Ni	0.001024
		^{62}Ni	0.003260
		^{64}Ni	0.000835
CHNO	1.678	C-nat.	0.3112
		^{1}H	0.0279
		^{14}N	0.2934
		^{16}O	0.3675