TRANSPORT THROUGH DIFFUSIVE AND NON-DIFFUSIVE REGIONS, EMBEDDED OBJECTS, AND CLEAR LAYERS.

GUILLAUME BAL*

Abstract. This paper deals with the diffusion approximation of transport equations in diffusive domains with non-diffusive inclusions, such as embedded objects and clear layers, where classical diffusion is not valid. Generalized diffusion equations with suitable non-local interface conditions at the boundary of the inclusions are derived. The asymptotic convergence of the transport solution to the generalized diffusion solution is shown for two types of inclusions. Numerical experiments assess the accuracy of the generalized diffusion equation. Applications include the modeling of thin clear layers filled with cerebrospinal fluid within the human head. Near-infra-red spectroscopy is increasingly being used in medical imaging for monitoring certain properties of human tissues. The presence of thin clear layers hampers the use of classical diffusion. This difficulty can be overcome by using the generalized diffusion model presented in this paper.

Key words. waves in random media, transport equations, diffusion approximation, clear layers, diffuse tomography, medical imaging.

AMS subject classifications. 45K05 92C55 76R50

1. Introduction.

Linear transport is used to model the propagation of particles and of the energy density of waves in scattering media. The particle description arises in physical phenomena such as the propagation of neutrons in nuclear reactor physics or electrons or photons in radiotherapy [3, 14]. The wave description models the propagation of electromagnetic waves in turbulent atmospheres and of shear waves in the Earth during an earthquake [11, 18, 24, 25], for instance.

In practice, transport equations are seldom solved numerically because they are posed in the phase space (the space of positions and velocities) and hence quite expensive. Instead, they are often approximated by diffusion equations, which are posed in the physical space and therefore computationally much cheaper. Moreover, diffusion equations capture by their very definition the macroscopic behavior of transport when the mean free path, the main distance between successive collisions of the particles with the passive underlying medium, is small. This can require substantial additional effort for the transport equation [7, 16, 21]. These observations encourage the use of diffusion whenever possible.

The transition from transport to diffusion is well-documented. Typically, as a particle travels though a scattering medium, its large time behavior resembles that of Brownian motion, whose probability density solves a diffusion equation. We refer to [9, 10, 13, 20] for classical references on the subject. Also well-known is the invalidity of the diffusion approximation in the vicinity of boundaries or interfaces shared with a non-scattering domain. Since the diffusion approximation is valid away from the interfaces, some mechanism has to explain the transition between the non-diffusive and diffusive behaviors. In the case of boundaries, this mechanism is mathematically well-understood [5, 8, 9, 13].

No such general theory exists in the presence of interfaces or non-scattering inclusions, although we refer to [6] for the analysis of a specific case in the one dimensional setting of interfaces of discontinuity. This paper aims at showing that macroscopic equations can still be derived even though diffusion breaks down within the inclu-

*Department of Applied Physics & Applied Mathematics, Columbia University, New York, NY 10027 USA, gb2030@columbia.edu

sions. Two main classes of inclusions are considered. The first one concerns large non-diffusive objects and the second one extended regions of relatively small volume such as clear layers.

An important application can be found in imaging through turbid media, for instance imaging of tumors or monitoring of cerebral oxygenation and haemodynamics using non-destructive near-infra-red (NIR) photons migrating in biological tissues. This field of research is currently very active in medical imaging [3, 4, 15, 17, 23]. One of the challenges of this technique consists in modeling the photon propagation inside a thin layer filled with cerebrospinal fluid (CSF), which is almost transparent to NIR photons, a few millimeters below the skull. This non-scattering and non-absorbing extended object has a major influence on the distribution of light inside the head, which classical diffusion completely fails to predict. This difficulty can be overcome by using the generalized diffusion model presented in this paper.

The paper is organized as follows. Section 2 gives the appropriate scaling of transport that leads to diffusion. The derivation of the diffusion equation, based on asymptotic techniques used in subsequent sections, is recalled. Section 3 deals with embedded objects that are large compared to the mean free path. The main results are the generalized diffusion equations for the leading term (3.2)-(3.4). Section 4 addresses the case of extended thin clear layers. The main result is the asymptotic convergence of the transport solution to the solution of a diffusion equation with non-local interface conditions provided that the thickness $L = L(\varepsilon)$ of the clear layer scales as $L^2|\ln L| \sim \varepsilon$, where ε is the mean free path in the diffusive domain. Finally, section 5 provides some numerical evidence that the diffusion model with non-local interface conditions is an accurate description of the transport solution in the simplified geometry of straight clear layers.

2. Transport Equation and Diffusion Approximation. The phase space particle density $u(x,v) = u(x,v;\varepsilon)$ solves the following transport equation [14]

$$\begin{aligned}&\frac{1}{\varepsilon} v\cdot\nabla u(x,v) + \frac{1}{\varepsilon^2}Q(u)(x,v) + \sigma_a(x)u(x,v) = S(x) \quad \text{in } \Omega\times V,\\ &u(x,v) = g(x,v) \quad \text{on } \Gamma_- = \{(x,v)\in\partial\Omega\times V \text{ s.t. } v\cdot\nu(x) < 0\}.\end{aligned} \tag{2.1}$$

Here, Ω is the physical domain, a regular open bounded subdomain in $\mathbb{R}^n$ where $n = 2,3$ is the space dimension, and V is the velocity domain, a closed bounded subdomain in $\mathbb{R}^n$. Typically, V is a finite union of spheres centered at $v = 0$ with classical surface measure $d\mu(v)$, or the finite union of coronas (a corona being the volume between two spheres centered at $v = 0$) with classical Lebesgue measure. We normalize μ such that $\mu(V) = 1$. It is also assumed that $0 \notin V$. The absorption coefficient is denoted by σ_a and the scattering operator defined by

$$Q(u)(x,v) = \sigma_s(x)\Big(u(x,v) - \int_V f(v',v)u(x,v')d\mu(v')\Big), \tag{2.2}$$

where the scattering coefficient $\sigma_s(x)$ is bounded and non-negative, and $f(v',v)$ is a bounded positive function satisfying

$$\int_V f(v,v')d\mu(v') = 1 \quad \text{for all } (x,v)\in\Omega\times V.$$

The absorption coefficient and scattering operator describe the interaction of the particles with the underlying medium. Classical assumptions are that σ_a and f are regular and non-negative, and σ_s is uniformly bounded from below by a positive constant. We also assume the reciprocity relation $f(v, v') = f(v', v)$.

The source terms are $S(x)$ and $g(x, v)$. The first one is the volume particle creation, a smooth function on Ω. The second one is the flux of particles entering the domain Ω through its boundary $\partial\Omega$. It is a smooth function on Γ_-, the set of incoming boundary conditions. The vector $\nu(x)$ denotes the outward normal to Ω at $x \in \partial\Omega$. Under these conditions, the transport equation (2.1) admits a unique solution in the Hilbert space $W^2(\Omega \times V)$ of functions $u(x, v)$ in $L^2(\Omega \times V)$ such that $v \cdot \nabla u(x, v)$ also belongs to $L^2(\Omega \times V)$ [2, 13].

The parameter ε measures the *mean free path*, the mean distance between two successive interactions of a particle with the medium. Mean free paths of order one are characteristic of the transport regime. Typically, particles undergo a finite number of scatterings before leaving the domain or being absorbed. When the mean free path and absorption coefficient are small, or equivalently when scattering is strong and absorption weak, particles undergo a large number of interactions with the medium before leaving Ω or being absorbed. Thus, original directional information is lost through scattering and the transport equation is well-approximated by its diffusive limit. The transport equation (2.1) is scaled so that the limit $\varepsilon \to 0$ corresponds to the diffusion regime.

We now delineate the steps of the derivation of the diffusion equation that will be important in subsequent sections. We follow the presentation in [13]. As $\varepsilon \to 0$, the number of interactions per unit length of the propagating particles with the underlying medium is of order ε^{-1} and the number of absorbed particles per unit distance of propagation is of order ε. The sources are also scaled so that the solution u remains bounded independently of ε. More precisely, when $g = 0$, we have [2, 5]

$$\|u\|_2 + \|v \cdot \nabla u\|_2 \leq C\|S\|_2, \tag{2.3}$$

where C is a constant independent of ε and $\|\cdot\|_p$ is the usual norm on $L^p(\Omega \times V)$. Further, assuming $S = 0$, we have the maximum principle [13]

$$\|u\|_\infty \leq C\|g\|_{L^\infty(\Gamma_-)}. \tag{2.4}$$

Here, the constant C is also independent of ε.

Whereas the diffusion approximation holds away from boundaries as a result of multiple scattering, it is not valid in the vicinity of the boundary. The asymptotic analysis of u requires two separate components. The first one describes the transport of particles far away from the boundary and is asymptotically described by the solution of the diffusion equation. The second component gives the transport solution in the vicinity of the boundary $\partial\Omega$. Since $\partial\Omega$ is smooth,

$$\hat{x} \in \partial\Omega \qquad \text{and} \qquad y = (\hat{x} - x) \cdot \nu(\hat{x})$$

form a coordinate system $x = (\hat{x}, y)$ for the points x in the vicinity of the boundary.

We consider the following asymptotic expansion for u

$$\begin{aligned} u(x, v) \quad = \quad & u_0(x, v) + \varepsilon u_1(x, v) + \varepsilon^2 u_2(x, v) + \varepsilon^3 u_3(x, v) + \zeta(x, v) \\ & + b^0\Big(\frac{\hat{x} - x}{\varepsilon}\nu(\hat{x}), v; \hat{x}\Big) + \varepsilon b^1\Big(\frac{\hat{x} - x}{\varepsilon}\nu(\hat{x}), v; \hat{x}\Big). \end{aligned} \tag{2.5}$$

Here, u_i is the ith term of the volume component. The terms b^i are boundary layers: they are concentrated in the vicinity of the boundary. More specifically, $b^i(\eta, v; \hat{x})$

decays exponentially as $\eta \to \infty$. To simplify notation, we shall write $b^i(\eta, v) = b^i(\eta, v; \hat{x})$ when no confusion is possible. The last term $\zeta(x, v)$ is a small corrector that will turn out to be of order ε^2.

2.1. Volume Asymptotic Expansion. We now plug the ansatz (2.5) into the transport equation (2.1) and equate like powers of ε. Concentrating on the volume component for the moment, we obtain the four equations

$$\begin{array}{llrcl} & \text{Order } \varepsilon^{-2}: & Q(u_0) & = & 0 \\ (2.6) & \text{Order } \varepsilon^{-1}: & v \cdot \nabla u_0 + Q(u_1) & = & 0 \\ & \text{Order } \varepsilon^{0}: & v \cdot \nabla u_1 + Q(u_2) + \sigma_a u_0 & = & S \\ & \text{Order } \varepsilon^{1}: & v \cdot \nabla u_2 + Q(u_3) + \sigma_a u_1 & = & 0. \end{array}$$

By assumption on $f(v, v')$, we see that $Q(1) = 0$. It follows from the Krein-Rutman theory [13] that 1 is the unique non-trivial solution to the equation $Q(u) = 0$. Therefore, we deduce that $u_0(x, v) = u_0(x)$.

Still from the Krein Rutman theory, we deduce the existence of a unique function $\theta_i(v) \in L^\infty(V)$, for $1 \le i \le n$, such that

$$\frac{1}{\sigma_s(x)} Q(\theta_i) = v_i, \qquad \int_V \theta_i(v) d\mu(v) = 0. \tag{2.7}$$

Introducing the vector $\theta = (\theta_1, \ldots, \theta_n)$, the first order corrector, obtained by solving the second equation in (2.6), is thus given by

$$u_1(x, v) = \frac{-1}{\sigma_s(x)} \theta \cdot \nabla u_0(x) + u_{10}(x), \tag{2.8}$$

where u_{10} has to be determined, but is independent of v. There is no analytic solution to (2.7) for general scattering operators. However, whenever $\int_V f(v, v') v' d\mu(v') = 0$, as in the isotropic case $f \equiv 1$ when V is a union of spheres and coronas, we check that $\theta(v) = v$.

The third equation admits a solution if and only if the Fredholm alternative holds:

$$\int_V (v \cdot \nabla u_1(x, v) + \sigma_a(x) u_0(x)) d\mu(v) = \int_V S(x) d\mu(v).$$

This relation is equivalent to the diffusion equation

$$-\text{div} D(x) \cdot \nabla u_0(x) + \sigma_a(x) u_0(x) = S(x) \quad \text{in } \Omega. \tag{2.9}$$

The diffusion tensor $D(x)$ of components $D_{ij}(x)$, $1 \le i, j \le n$ is given by

$$D_{ij}(x) = \frac{1}{\sigma_s(x)} \int_V v_i \theta_j(v) d\mu(v). \tag{2.10}$$

It is uniformly positive definite (see [13]), which ensures that the diffusion equation (2.9) with appropriate boundary conditions is well-posed.

Solving the third equation in (2.6) for u_2 and using the compatibility condition of the fourth equation in (2.6) yields similarly (see [13]) that

$$-\text{div} D(x) \cdot \nabla u_{10}(x) + \sigma_a(x) u_{10}(x) = 0 \quad \text{in } \Omega. \tag{2.11}$$

We have so far obtained equations for u_0 and u_1 in (2.5). Additional equations for u_2 and subsequent terms could be obtained by carrying on the same procedure to higher orders.

2.2. Boundary Layers. We now turn to the boundary layer terms, and plug the ansatz (2.5) into the boundary conditions for the transport equation (2.1). For $(\hat{x}, v) \in \Gamma_-(\Omega)$, we obtain the following equations:

$$\begin{array}{lrcl} \text{Order } \varepsilon^0 : & u_0(\hat{x}) + b^0(0, v; \hat{x}) & = & g(\hat{x}, v), \\ \text{Order } \varepsilon^1 : & -\dfrac{1}{\sigma_s(\hat{x})}\theta \cdot \nabla u_0(\hat{x}) + u_{10}(\hat{x}) + b^1(0, v; \hat{x}) & = & 0. \end{array} \tag{2.12}$$

It is clear from these two equations that boundary layer terms are necessary to justify the asymptotic expansion in the volume. Indeed, the first continuity condition in (2.12) cannot be satisfied without $b^0(0, v; \hat{x})$ when $g(\hat{x}, v)$ is non-trivial in v. Since u_{10} is independent of v, the second continuity condition also cannot be satisfied without the boundary layer term $b^1(0, v; \hat{x})$.

However, the asymptotic expansion developed in the previous section has to hold in the volume, that is far away from the boundary. Hence, the boundary layer terms have to decay rapidly away from the boundary. Equations for the boundary layer terms are obtained from the transport equation (2.1) by magnifying the boundary layer in the vicinity of a point $\hat{x} \in \partial\Omega$. Upon plugging $b(\eta, v; \hat{x})$ with $\eta = \varepsilon^{-1}(\hat{x} - x)\nu(\hat{x})$ into (2.1) and sending $\varepsilon \to 0$, we obtain in the limit that

$$v \cdot \nu(\hat{x}) \frac{\partial b^k(\eta, v)}{\partial \eta} + Q(b^k)(\eta, v) = 0 \qquad (\eta, v) \in \mathbb{R}^+ \times V, \tag{2.13}$$

for $k = 0, 1$. The well-posedness of this equation supplemented with suitable boundary conditions is treated in the following lemma [5, 8, 13].

LEMMA 2.1. *Let $\hat{x} \in \partial\Omega$ and $V_- = \{v \in V \text{ s.t. } v \cdot \nu(\hat{x}) < 0\}$. For all $g \in L^\infty(V_-)$, there is a unique solution $b(\eta, v) \in L^\infty(\mathbb{R}^+ \times V)$ to (2.13) with the boundary condition $b(0, v) = g(v)$ on V_-. Moreover, b converges exponentially to a constant $\Lambda(g)$, where $\Lambda = \Lambda(\hat{x})$ is a linear form on $L^\infty(V_-)$, depending on the scattering operator Q at $\hat{x}$.*

The outgoing distribution $b(0, v)$ is in $L^\infty(V_+)$ where $V_+ = \{v \in V \text{ s.t. } v \cdot \nu(\hat{x}) > 0\}$. We denote by $\mathcal{R} = \mathcal{R}(\hat{x})$ the response operator mapping g in $L^\infty(V_-)$ to $b(0, v)$ in $L^\infty(V_+)$:

$$\mathcal{R} : \begin{array}{l} L^\infty(V_-) \to L^\infty(V_+) \\ g \mapsto \mathcal{R}(g) = b(0, \cdot). \end{array} \tag{2.14}$$

We deduce from the lemma that

$$u_0(\hat{x}) = \Lambda(g(\hat{x}, v)) \tag{2.15}$$

is the only boundary condition for u_0 that is compatible with the exponential decay of b^0. Indeed, $b^0(\eta, v)$ decays exponentially when $\Lambda(b^0(0, v)) = 0$, that is to say, thanks to (2.12), when $\Lambda(g(\hat{x}, v) - u_0(\hat{x})) = 0$ which is (2.15) since $\Lambda(1) = 1$. Similarly, the boundary condition that allows b^1 to decay exponentially is

$$u_{10}(\hat{x}) = \frac{1}{\sigma_s(\hat{x})} \Lambda(\theta) \cdot \nabla u_0(\hat{x}) = \Lambda(\theta \cdot \nu(\hat{x})) \frac{1}{\sigma_s(\hat{x})} \frac{\partial u_0}{\partial \nu(\hat{x})}. \tag{2.16}$$

The latter equality is deduced from symmetry relations. We can show [13] that the *extrapolation length*

$$L = \Lambda(-\theta \cdot \nu(\hat{x})) \tag{2.17}$$

is positive. An approximate value when $f \equiv 1$ is $L \approx 0.7104$ when the space dimension $n = 3$. There exist several studies on the linear form Λ and the extrapolation length for various scattering kernels $f(v, v')$; see for instance the review article [26] and its references.

2.3. Diffusion Equation. Let us summarize the calculations presented in the two previous subsections. We have obtained that

$$\begin{aligned} u(x,v) &= u_0(x) + b^0\Big(\frac{x-\hat{x}}{\varepsilon}, v\Big) \\ &+ \varepsilon\Big(u_{10}(x) - \frac{1}{\sigma_s(x)}\theta\cdot\nabla u_0 + \varepsilon b^1\Big(\frac{x-\hat{x}}{\varepsilon}, v\Big)\Big) + O(\varepsilon^2). \end{aligned} \tag{2.18}$$

The volume terms u_0 and u_{10} satisfy the following diffusion equations

$$\left\{\begin{array}{l} -\mathrm{div} D(x)\cdot\nabla u_0(x) + \sigma_a(x) u_0(x) = S(x) \quad \text{in} \quad \Omega \\ u_0(x) = \Lambda(g(x,v)) \qquad \text{on} \quad \partial\Omega. \end{array}\right. \tag{2.19}$$

$$\left\{\begin{array}{l} -\mathrm{div} D(x)\cdot\nabla u_{10}(x) + \sigma_a(x) u_{10}(x) = 0 \quad \text{in} \quad \Omega \\ u_{10}(x) = -L\dfrac{1}{\sigma_s(x)}\dfrac{\partial u_0}{\partial\nu(x)} \qquad \text{on} \quad \partial\Omega. \end{array}\right. \tag{2.20}$$

The positive definite diffusion tensor $D(x)$ is given by (2.10). The extrapolation length L is positive.

In practice, the boundary layer terms b^0 and b^1 are not computed explicitly. Since they decay exponentially, we deduce that $\|b^k(\varepsilon^{-1}(x-\hat{x}), v)\|_p \leq C\varepsilon^{1/p}$ for $1 \leq p \leq \infty$. Moreover, they are negligible for every point x away from the boundary. A proof that the error in (2.18) is indeed of order ε^2 can be found in [13].

This paper only presents the steady-state case to simplify. However, incorporating time dependence is straightforward. At the transport level, an additional term $\partial_t u(x,v)$ is present on the left hand side of (2.1). In the diffusive regime, this translates into adding the terms $\partial_t u_0$ and $\partial_t u_{10}$ on the left hand side of (2.19) and (2.20), respectively; see [13] for the details. The diffusion equations in the following sections are modified accordingly.

3. Embedded Non-diffusive Objects. We now consider the first class of non-scattering inclusions. Let Ω be an open convex bounded subdomain in $\mathbb{R}^n$ and Ω^C an open smooth subdomain embedded in Ω. We denote by $\Omega^E = \Omega\backslash\overline{\Omega^C}$ the complementary of Ω^C in Ω (see Fig. 3.1). We assume that Ω^E is diffusive and that Ω^C is not. The transport equation is then given by

$$\begin{array}{l} \dfrac{1}{\varepsilon}v\cdot\nabla u(x,v) + \dfrac{1}{\varepsilon^2}Q(u)(x,v) + \sigma_a(x)u(x,v) = S(x) \quad \text{in} \quad \Omega^E\times V \\ u(x,v) = g(x,v) \qquad \text{on} \quad \Gamma_- \\ v\cdot\nabla u^c(x,v) + Q^c(u^c)(x,v) + (\sigma_{a0}+\varepsilon\sigma_{a1})u^c(x,v) = 0 \quad \text{in} \quad \Omega^C\times V \\ u(x,v) = u^c(x,v) \qquad \text{on} \quad \partial\Omega^C\times V. \end{array} \tag{3.1}$$

In this section, the domain Ω^C is independent of ε. Hence, in the limit $\varepsilon \to 0$, the object in this model is large compared to the mean free path of the diffusive region. The following result shows the non-local influence of the embedded object on the transport equation in the diffusive regime.

The solution u in the coupled problem (3.1) converges to u_0 (strongly in $L^2(\Omega^E\times V)$) with an error of order ε (in the same norm), where u_0 solves the following diffu-

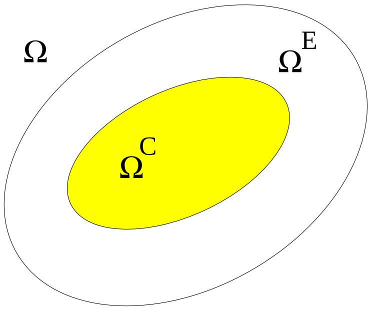

FIG. 3.1. *Geometry of Embedded object.*

sion equation

$$-\text{div} D(x) \cdot \nabla u_0(x) + \sigma_a(x) u_0(x) = S(x) \qquad in \quad \Omega^E \tag{3.2}$$
$$u_0(x) = \Lambda(g(x,v)) \qquad on \quad \partial\Omega.$$

The coefficient D is given by (2.10) and the form Λ by Lemma 2.1. We distinguish two cases.

- *Assume that $\sigma_{a0} > 0$. Then, we have*

$$u_0 = 0 \qquad on \quad \partial\Omega^C. \tag{3.3}$$

- *Assume that $\sigma_{a0} = 0$. Then the conditions at the boundary $\partial\Omega^C$ are*

$$u_0(x) = \text{Constant} \qquad on \quad \partial\Omega^C \tag{3.4}$$
$$\int_{\partial\Omega^C} \nu_E^t \cdot D(x) \cdot \nabla u_0 \, d\sigma(x) + u_{0|\partial\Omega^C} \int_{\Omega^C} \sigma_{1a}(y) dy = 0.$$

We now derive this result. The ansatz (2.5) holds for u and we write $u^c(x,v) = u_0^c(x,v) + \varepsilon u_1^c(x,v) + \zeta^c(x,v)$. Equating like powers of ε yields

$$v \cdot \nabla u_0^c + Q^c(u_0^c) + \sigma_{a0} u_0^c = 0 \qquad \text{in} \quad \Omega^C \times V \tag{3.5}$$
$$u_0(x) + b^0(0,v) = u_0^c(x,v) \qquad \text{on} \quad \partial\Omega^C \times V.$$

Let us assume that the source terms S and g are positive. Then, by positiveness of the transport equation, the solution (u, u^c) is also positive. Let us integrate the first equation in (3.5) over $\Omega^C \times V$. By integrations by parts, we get that

$$\int_{\partial\Omega^C \times V} v \cdot \nu(x) u_0^c d\sigma(x) d\mu(v) + \int_{\Omega^C \times V} \sigma_{a0} u_0^c dx d\mu(v) = 0.$$

Using the boundary condition in (3.5) and recalling that $\int_V v \cdot \nu(x) b^0 d\mu(v) = 0$ because b^0 solves (2.13), we obtain that

$$\int_{\Omega^C \times V} \sigma_{a0} u_0^c(x,v) dx d\mu(v) = -\int_{\partial\Omega^C \times V} v \cdot \nu(x) u_0^c d\sigma(x) d\mu(v) = 0.$$

Since u_0^c is non-negative as the limit of non-negative functions u^c, we deduce that $u_0^c \equiv 0$ when σ_{a0} is positive, and by continuity that $u_0 = 0$ on $\partial\Omega^C$. This is condition (3.3).

Let us now assume $\sigma_{a0} = 0$. We easily observe that $u_0 = u_0^c =$ Constant clearly solves (3.5). Using techniques similar to those in [5, 6], we can show that constants are actually the only solutions of (3.5). This is the condition of global equilibrium given as the first equation in (3.4).

The term of order ε is given by

$$\begin{aligned} v \cdot \nabla u_1^c + Q^c(u_1^c) + \sigma_{a1} u_0^c = 0 \qquad & \text{in} \quad \Omega^C \times V, \\ u_1(x,v) + b^1(0,v) = u_1^c(x,v) \qquad & \text{on} \quad \partial\Omega^C \times V. \end{aligned} \tag{3.6}$$

Let us again integrate this equation over $\Omega^C \times V$. Similarly to what we have obtained above, we get that

$$\int_{\partial\Omega^C \times V} v \cdot \nu(x) u_1(x,v) d\sigma(x) d\mu(v) + u_0^c \int_\Omega \sigma_{a1}(x) dx = 0,$$

because $u_0^c = u_0$ is now constant on $\partial\Omega^C$. Replacing u_1 by its expression in (2.8) yields the second condition in (3.4). The latter condition is actually the compatibility condition that ensures the existence of solutions to (3.6). The rigorous proof of this assertion requires more involved techniques than the integrations by parts presented above and is not considered here. Again, this result can be made rigorous by using techniques similar to those in [5, 6].

The main result of this section is the interface conditions (3.4). Since the object is large compared to the mean free path of the diffusive domain and the mean free path inside the object is of order one, the particles entering the domain Ω^C can freely cross the object; hence enforcing the condition that u_0 is constant on $\partial\Omega^C$. When the object is weakly absorbing, the current of particles crossing Ω^C is damped by an amount given by the second interface condition, which expresses the conservation of the flux of particles across the inclusion.

Let us conclude this section with a remark on the 'classical' diffusion approximation treated in section 2. The transport equation (3.1) on $\Omega^C \times V$ has the same form as on $\Omega^E \times V$ when $\sigma_{a0} = 0$ provided we replace σ_s by $\varepsilon\sigma_s$. If we used the diffusion approximation of section 2 on Ω^C, we would obtain a diffusion tensor (2.10) inversely proportional to the scattering cross section, hence of order ε^{-1}. Now assuming that (2.9) holds on Ω^C as well with a diffusion tensor of order ε^{-1} and letting $\varepsilon \to 0$ in this diffusion equation posed on the full domain Ω leads to the same limit (3.2)-(3.4). This is most easily checked in the variational formulation of (2.9). Consequently, although the 'classical' diffusion equilibrium $-u_0(x,v)$ is independent of $v-$ is modified in the case of non-scattering inclusions $-u_0(x)$ is constant over $\partial\Omega^C$; the equilibrium is non-local in space–, the classical diffusion approximation (2.9) is as good an approximation to the transport equation (3.1) as (3.2)-(3.4) is. We will see that such is not the case when thin clear layers are present.

4. Clear Layers. This section addresses the case of extended non-diffusive regions such as clear layers. We model the clear layer as follows (see Fig. 4.1). Let Ω^I be an open subdomain of Ω. We define $\Sigma = \partial\Omega^I$ and the clear layer $\Omega^C = \Omega^C(\varepsilon)$ by

$$\Omega^C = \{y \in \Omega \text{ such that } \quad y = x + t\nu(x), \quad \text{where } x \in \Sigma,\ |t| < lL\}, \tag{4.1}$$

where $\nu(x)$ is the outward unit normal vector to Ω^I at $x \in \Sigma$, $L = L(\varepsilon)$ is the non dimensional mean thickness of the clear layer, which depends on the mean free path ε, and l is a positive length. We assume that $\Omega^C \subset \Omega$ for L small enough.

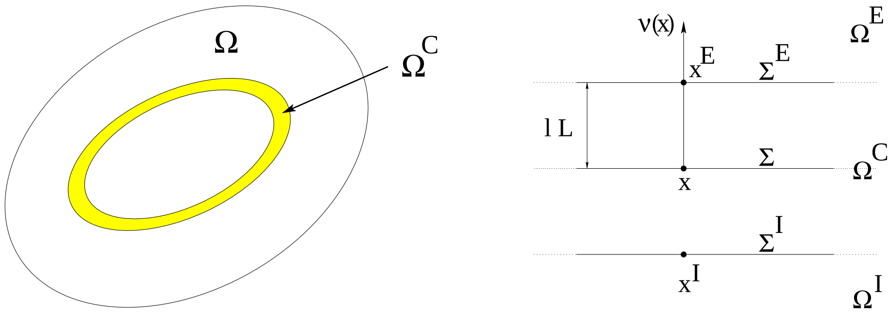

FIG. 4.1. *Left: Geometry of the clear layer. The external and internal regions* $\Omega\backslash\Omega^C$ *are diffusive, whereas the clear layer* Ω^C *is not. Right: Local Geometry of the clear layer near a point* $x \in \Sigma \subset \Omega^C$.

When L is chosen independent of ε, the clear layer Ω^C is nothing but a large inclusion, and the results of the preceding section apply. Therefore, the effect of a large non-diffusive and weakly absorbing layer is to force a constant particle density at the boundary $\partial\Omega^C$. As a consequence, the particle density is asymptotically constant in the whole internal domain Ω^I. Notice that no object inside Ω^I can be detected at this order of approximation, since the diffusion approximation only depends on the physical data in $\Omega^E = \Omega\backslash\Omega^I$. A thick clear layer inside a diffusive medium will then be a very efficient screen and hamper the use of diffuse tomography as an imaging technique.

The physics is different when L becomes small as $\varepsilon \to 0$, that is to say when the layer is thin in one direction and thick in the other directions. A particle reaching one side of Ω^C has a twofold behavior, depending on its normal velocity $v \cdot \nu(x)$. When $v \cdot \nu(x)$ is large, the particle crosses the layer through its thin section and reenters the diffusive region as if there were no layer. When $v \cdot \nu(x)$ is close to 0 however, the particle can propagate across the layer for a much longer time and trigger a non-local influence. Since the particle density in the diffusive regime is relatively uniform in the velocity variable, most particles reaching the boundary $\partial\Omega^C$ have a normal velocity far from 0, hence behave as if the thin layer did not exist. Consequently, the diffusive equilibrium will not break down and u_0 will remain approximately continuous across the clear layer. However, for layers that are not too thin, the density of particles traveling for a long time across the layer is sufficiently large to influence the relationship between the particle density u_0 and its flux $D\partial_\nu u_0$ across the interface Σ. This section aims at deriving a new relationship between u_0 and $D\partial_\nu u_0$ across the clear layer that takes into account the non-diffuseness and the geometry of the inclusion. A non trivial relationship that differs from those of the previous sections will be obtained when the clear layer thickness L scales as $L^2|\ln L| = \varepsilon$. When L is smaller, the leading term in the transport equation does not 'see' the clear layer and we obtain the classical diffusion approximation (2.19). When L is larger, the layer is too thick to accommodate a local diffusive regime, and we come back to the case of a large inclusion (3.4) as in the preceding section.

4.1. Derivation of the modified diffusion equation. The transport equation can be written as the following coupled problem

$$
\begin{aligned}
&\frac{1}{\varepsilon} v\cdot\nabla u + \frac{1}{\varepsilon^2} Q(u) + \sigma_a(x) u = S(x) \quad \text{in } (\Omega\backslash\Omega^C)\times V\\
&u = g \quad \text{on } \Gamma_-\\
&v\cdot\nabla u^c + \sigma_a^c u^c + Q^c(u^c) = 0 \qquad \text{in } \Omega^C\times V\\
&u = u^c \quad \text{on } \partial\Omega^C\times V.
\end{aligned} \tag{4.2}
$$

It is convenient to replace the transport equation inside the clear layer Ω^C by the response operator $\mathcal{R}^c = \mathcal{R}^c(\varepsilon)$ that maps the incoming distribution on Γ_-^C to the outgoing distribution $\Gamma_+^C = \{(x,v)\in\partial\Omega^C\times V \text{ s.t. } v\cdot\nu(x)>0\}$. We then recast (4.2) as

$$
\begin{aligned}
&\frac{1}{\varepsilon} v\cdot\nabla u + \frac{1}{\varepsilon^2} Q(u) + \sigma_a(x) u = S(x) \quad \text{in } (\Omega\backslash\Omega^C)\times V\\
&u = g \quad \text{on } \Gamma_-\\
&u = \mathcal{R}^c(u) \quad \text{on } \Gamma_+^C.
\end{aligned} \tag{4.3}
$$

We are interested in the case where the clear layer is thin enough so as not to modify the local diffusive equilibrium. Therefore, we are in a situation where the operator $\mathcal{R}^c$ can be written asymptotically as

$$\mathcal{R}^c = \mathcal{I} + \varepsilon\mathcal{R}_1^c, \tag{4.4}$$

where the operator $\mathcal{I}$ is a near identity operator. Let us introduce some notation (see also Fig. 4.1). We denote by $\Gamma_\pm^{CX}$ the subsets of $\Gamma_\pm^C$ that are physically on Σ^X for $X = E, I$, where the outer and inner surfaces are defined by

$$\Sigma^E = \Sigma + lL\nu(x), \qquad \Sigma^I = \Sigma - lL\nu(x). \tag{4.5}$$

For any function $u(x,v)\in\partial\Omega^C\times V$, we denote similarly by $u^X(x,v)$ its restriction on Σ^X for $X = E, I$. For every point $x\in\Sigma$, we define

$$x^I = x - lL\nu(x) \qquad \text{and} \qquad x^E = x + lL\nu(x). \tag{4.6}$$

The operator $\mathcal{I}$ is a translation operator, which, like $\mathcal{R}^c$, maps Γ_-^C to Γ_+^C. It is defined on Γ_-^{CE} and Γ_-^{CI} by

$$\mathcal{I}u(x,v) = \left\{\begin{array}{ll} \mathcal{I}^E u^E(x,v) = u^E(x+2lL\nu(x),v) & (x,v)\in\Gamma_-^{CI},\\ \mathcal{I}^I u^I(x,v) = u^I(x-2lL\nu(x),v) & (x,v)\in\Gamma_-^{CE}. \end{array}\right. \tag{4.7}$$

Notice that by construction of the clear layer, $\nu_E(x^E) = \nu(x) = -\nu_I(x^I)$ for every $x\in\Sigma$, where ν_E and ν_I are the outward unit normals to Ω^C on Σ^E and Σ^I, respectively. One then checks that $\mathcal{I}$ maps Γ_-^C to Γ_+^C, and more specifically, $\mathcal{I}^E$ maps Γ_-^{CE} to Γ_+^{CI} and $\mathcal{I}^I$ maps Γ_-^{CI} to Γ_+^{CE}. For $x\in\Sigma^I$, we define the change of variables $y(x) = x + 2lL\nu(x)$ and denote by $J(x) = J(x;\varepsilon)$ the Jacobian of the transformation

$$J(x) = |\det(I + 2lL\nabla_x\nu(x))|. \tag{4.8}$$

An important part of the analysis of clear layers is to figure out which thickness L of the clear layer renders the operator $\mathcal{R}_1^c$ in (4.4) of order one when it is applied to functions that only depend on the spatial variable. This will be done in the following subsections for specific clear layers. For now, we assume that the decomposition (4.4) makes sense and obtain a modified diffusion equation that takes into account the clear layer. The following result characterizes the non-local effects of the clear layer.

Assume that the operator $\mathcal{R}_1^c$ above applied to sufficiently smooth functions of x is of order one (say in $L^\infty(\Gamma_+^C)$). The solution u of the coupled problem (4.2) is then approximated, up to an error of order ε, by the solution $u_0 = u_0(\varepsilon)$ of the following ε-dependent diffusion equation

$$\begin{aligned} &-\mathrm{div} D(x)\cdot\nabla u_0(x) + \sigma_a(x)u_0(x) = S(x) \qquad \text{in } \Omega\backslash\Omega^C \\ &u_0(x) = \Lambda(g(x,v)) \qquad \text{on } \partial\Omega \\ &[[u_0]] = 0 \qquad \text{on} \quad \Sigma^E \\ &[\nu\cdot D\nabla u_0] = K(u_0) \qquad \text{on} \quad \Sigma^E, \end{aligned} \tag{4.9}$$

where the jump conditions are defined by

$$[[u]](x^E) = u(x^E) - u(x^I) \qquad \text{and} \qquad [u](x^E) = u(x^E) - J(x^I)u(x^I), \tag{4.10}$$

and the integral operator $K = K(\varepsilon)$ is given by

$$\begin{aligned} Ku(x^E) \;&=\; \int_{v\cdot\nu_E(x^E)>0} v\cdot\nu_E(x^E)\,(\mathcal{R}_1^c u)(x^E,v)d\mu(v) \\ &+\; J(x^I)\int_{v\cdot\nu_I(x^I)>0} v\cdot\nu_I(x^I)\,(\mathcal{R}_1^c u)(x^I,v)d\mu(v) \qquad x^E\in\Sigma^E. \end{aligned} \tag{4.11}$$

Since u_0 is continuous across the layer, we identify $u_0(x^E) = u_0(x^I)$ for $x^E \in \Sigma^E$. The difference between the two jump operators $[[\cdot]]$ and $[\cdot]$ becomes small as $\varepsilon \to 0$ since, as we shall see in the next section, $L \to 0$ as $\varepsilon \to 0$. However, while the former indicates that the diffusion equilibrium is not perturbed, the latter ensures the conservation of the flux of particles across the layer Ω^C; hence involves the Jacobian of the near-identity transformation $\mathcal{I}$.

We now underline the main steps of the derivation of (4.9). The asymptotic expansion (2.18) holds inside the domain $\Omega\backslash\Omega^C$ and we would like it to hold also in the vicinity of Ω^C. Plugging (2.18) into the boundary conditions of (4.3) on Γ_+^C, using (4.4), and equating like powers of ε yields at the order ε^0 that

$$u_0 + b^0 = \mathcal{I}\mathcal{R}(u_0 + b^0) \qquad \text{on} \quad \Gamma_+^C, \tag{4.12}$$

since $b^i{}_{|\Gamma_+^C} = \mathcal{R}b^i{}_{|\Gamma_-^C}$ and $u_0 = u_0(x)$. Let us introduce the vectorial notation $b = (b^I, b^E)$ for every function defined on Γ_-^C. Then the above problem can be recast as

$$b = \begin{pmatrix} 0 & \mathcal{I}^E\mathcal{R} \\ \mathcal{I}^I\mathcal{R} & 0 \end{pmatrix} b. \tag{4.13}$$

By definition of $\mathcal{I}$, this problem is local at $(x^I, x^E = y(x^I))$. It is easily seen that $b = 1$ solves this equation, and it can be shown that it is the unique solution up to multiplication by a constant at $(x^I, x^E = y(x^I))$ fixed. Therefore, the unique solution to (4.12) is $u_0 = \mathcal{I}u_0$ and $b^0 = 0$ since we want this term to decay at infinity. This is equivalent to the first jump condition $u_0(x^E) = u_0(x^I)$.

The order ε reads

$$b^1 = \begin{pmatrix} 0 & \mathcal{I}^E\mathcal{R} \\ \mathcal{I}^I\mathcal{R} & 0 \end{pmatrix} b^1 + \begin{pmatrix} f^I \\ f^E \end{pmatrix}, \qquad \text{where} \tag{4.14}$$

$$f^I = \mathcal{I}^E u_1^E - u_1^I + \mathcal{R}_1^c u_0 \qquad \text{and} \qquad f^E = \mathcal{I}^I u_1^I - u_1^E + \mathcal{R}_1^c u_0. \tag{4.15}$$

This system admits a solution provided the Fredholm alternative holds, i.e. provided $f = (f^I, f^E)$ is orthogonal to the solution of the adjoint eigenvalue problem

$$b^* = \begin{pmatrix} 0 & \mathcal{R}^*\mathcal{I}^{I*} \\ \mathcal{R}^*\mathcal{I}^{E*} & 0 \end{pmatrix} b^*, \tag{4.16}$$

where $b^* = (b^{I*}, b^{E*})$. We then check that $\mathcal{I}^{E*} = J^{-1}(x)\mathcal{I}^I$ and $\mathcal{I}^{I*} = J(x)\mathcal{I}^E$. The problem is then local in (x^I, x^E) and the unique solution up to multiplication by a constant is

$$b^{E*}(v) = v \cdot \nu_E(x^E) \qquad \text{and} \qquad b^{I*}(v) = J(x^I) v \cdot \nu_I(x^I). \tag{4.17}$$

The compatibility condition for the solvability of (4.14) is therefore

$$J(x^I) \int_{v\cdot\nu_I(x^I)>0} v \cdot \nu_I(x^I) f^I(x^I) d\mu(v) + \int_{v\cdot\nu_E(x^E)>0} v \cdot \nu_E(x^E) f^E(x^E) d\mu(v) = 0. \tag{4.18}$$

From (4.15) and (2.8) for u_1 (with $u_{10} = 0$ since we are only interested in the leading term of the expansion), we obtain that (4.18) is equivalent to the second jump condition in (4.9).

Now that we have the diffusion equation (4.9), it remains to convince ourselves that it is well-posed. Assume again that the boundary condition g vanishes to simplify. The variational formulation of (4.9) reads

$$\int_{\Omega\backslash\Omega^C} (\nabla u_0 \cdot D\nabla u_0 + \sigma_a (u_0)^2) dx - \int_{\partial\Omega^C} D\nabla u_0 \cdot \nu(x) u_0 d\sigma = \int_{\Omega\backslash\Omega^C} u_0 S dx. \tag{4.19}$$

Here, $\nu(x)$ is the outward normal to $\partial\Omega^C$. Therefore, for $x^E \in \Sigma^E$, we have $\nu(x^E) = \nu_E(x^E)$ and for $x^I \in \Sigma^I$, $\nu(x^I) = -\nu_I(x^I)$.

Since u_0 is constant across the interface and the change of measure from Σ^E to Σ^I is $d\sigma_E(y) = J(x)d\sigma_I(x)$, we deduce from the interface condition that

$$\begin{aligned} &-D\nabla u_0 \cdot \nu_E(x^E) u_0 d\sigma_E - D\nabla u_0 \cdot \nu_I(x^I) u_0 d\sigma_I = -u_0 \tilde{K} u_0 d\sigma_E \\ &-(1-J^2) D\nabla u_0 \cdot \nu_I(x^I) u_0 d\sigma_I + (1-J) u_0 \Big[\int_{v\cdot\nu_I(x)>0} v \cdot \nu_I(x) \mathcal{R}_1^c u_0 d\mu(v) \Big] d\sigma_E, \end{aligned} \tag{4.20}$$

where $\tilde{K}$ has the same expression as K except that the term $J(x^I)$ is replaced by 1. Integrating the left hand side of this equation gives the boundary term in the variational formulation (4.19). The right-hand side is composed of three terms. We will see that the first term is positive, which is the right sign. The second and third terms are not necessarily positive, and could cause some difficulties in the variational formulation. Fortunately, they are small and dominated by the first term on the left-hand side of (4.19).

Let us first demonstrate that $\tilde{K}$ is non-negative. This is deduced from the properties of the response operator $\mathcal{R}^c$. Using the classical variational formulation of the transport equation (see [2] for instance), we deduce that

$$\int_{\Gamma_+^C} v \cdot \nu(x) \Big(\mathcal{R}^c u\Big)^2 d\sigma d\mu \le \int_{\Gamma_-^C} |v \cdot \nu(x)|\, u^2 \, d\sigma d\mu,$$

and by the Cauchy-Schwartz inequality $\int_{\Gamma_+^C} v \cdot \nu(x) u \mathcal{R}^c u d\sigma d\mu \le \int_{\Gamma_-^C} |v \cdot \nu(x)|\, u^2 \, d\sigma d\mu$. For those functions u satisfying $\mathcal{I}u = u$, we have

$$\int_{\Gamma_+^C} v \cdot \nu(x) u \, \mathcal{I} u \, d\sigma d\mu = \int_{\Gamma_-^C} |v \cdot \nu(x)|\, u^2 \, d\sigma d\mu.$$

Subtracting these last two relations shows that $\mathcal{R}_1^c$ is non-positive, therefore

$$-\int_{\Sigma^E} u_0 \tilde{K} u_0 d\sigma_E \geq 0.$$

Let us now show that the two remaining terms on the right-hand side of (4.20) are dominated by the first term on the left-hand side of (4.19). Indeed, as $\varepsilon \to 0$, $L \to 0$ and $J \to 1$ uniformly. We denote by $\eta = \eta(\varepsilon)$ the maximum of $|1-J|$ and $|1-J^2|$. Thus, we have

$$\begin{aligned}\int_{\Sigma^I} |(1-J^2)\nabla u_0 \cdot \nu_I(x^I) u_0| d\sigma_I &\leq C\eta \|\nabla u_0\|_{H^{-\frac{1}{2}}(\Sigma^I)} \|u_0\|_{H^{\frac{1}{2}}(\Sigma^I)} \\ &\leq C\eta \|u_0\|^2_{H^1(\Omega\backslash\Omega^C)},\end{aligned}$$

by classical trace inequality [1]. Since $\eta \to 0$ as $\varepsilon \to 0$, as soon as ε is small enough, this term is dominated by say one third of the first term in (4.19). Since $\mathcal{R}_1^c$ is bounded and by the Cauchy-Schwartz inequality, the second term is bounded by η times the $L^2(\Sigma^E)$-norm of u_0, therefore by η times its $H^1(\Omega\backslash\Omega^C)$-norm. So this term too is dominated by one third of the first term in (4.19) and the variational formulation ensures the existence of a unique solution $u_0 \in H^1(\Omega\backslash\Omega^C)$ to (4.9).

Notice that the variational formulation of the diffusion equation is well-posed only when L is small. In some sense, imposing $u_0 = \mathcal{I}u_0$ to the leading term is not a 'natural' variational condition for the diffusion equation, since the contraction from Σ^E to Σ^I is not taken into account. Yet the transport equation, posed in phase space, does not see this contraction. It is then not surprising that the notions of conservation of current crossing Ω^C differ for transport and diffusion. The jump conditions in the theorem ensure conservation of current at the transport level. As we have seen, this translates into a difficulty in the variational formulation of the diffusion equation. Notice also that as L grows larger, up to being of order 1, the asymptotic regime is governed by what is described in the results of section 3. There, the variational formulation for diffusion is well-posed, but the local condition $u_0 = \mathcal{I}u_0$ is no longer imposed.

4.2. Scaling of the clear layers. The results in the previous section are based on the validity of the expansion (4.4). This section derives the correct scaling that the clear layer must satisfy in order for (4.4) to hold. To simplify the derivation, we consider the space dimension $n = 2$ and assume that the clear layer is an annulus; i.e. the surface Σ is a circle of radius R. The generalization to clear layers of the form given in Fig. 4.1 and to higher space dimensions is straightforward. We will consider the case of straight layers in the next subsection. Since our main interest is to deal with *clear* layers, we assume that $Q^c \equiv 0$, and that the absorption coefficient σ_a^c is constant. We also suppose that $V = S^1$, the unit circle in $\mathbb{R}^2$.

Let $(x, v) \in \Gamma_+^C$. We write $v = (\cos\phi, \sin\phi)$. We denote by $t(x, \phi)$ the traveling time between x and $\partial\Omega^C$ in the direction $-v$, that is to say, the smallest positive real number such that $x - t(x,\phi)v \in \partial\Omega^C$. We also define $\bar{x} = \bar{x}(x,\phi) = x - t(x,\phi)v$. Solving the free transport equation along its characteristics, we obtain

$$\mathcal{R}^c u(x,\phi) = e^{-\sigma_a^c t(x,\phi)} u(\bar{x}). \tag{4.21}$$

We verify that the traveling time $t(x,\phi)$ is uniformly bounded by a constant times $\sqrt{L}$ for L small enough, as an application of the Pythagorean theorem. More precisely, for $x = x^I \in \Sigma^I$, the equation for t is $x^I - tv \in \Sigma^E$, i.e.,

$$(R - lL + t\sin\phi)^2 + t^2\cos^2\phi = (R + lL)^2.$$

Solving for $t > 0$ yields

$$\begin{aligned} t &= -(R-lL)\sin\phi + \sqrt{4lLR + (R-lL)^2\sin^2\phi} \\ &= (R-lL)\sin\phi\Big(\sqrt{1+\frac{\tau}{\sin^2\phi}} - 1\Big), \\ &= (R-lL)\Big(\frac{\tau}{2\sin\phi} - \frac{\tau^2}{8\sin^3\phi} + O(\frac{\tau^3}{\sin^5\phi})\Big), \end{aligned} \tag{4.22}$$

with $\tau = 4lLR/(R-lL)^2$. We observe that $t \sim 2l(\sin\phi)^{-1}L$ when $\sin\phi >> L$ and $t \sim 2\sqrt{lR}\sqrt{L}$ when $\sin\phi << L$. In any case, $t \leq 2\sqrt{lR}\sqrt{L}$ goes to 0 with L. Consequently, $\mathcal{R}^c u(x,v)$ for $(x,v) \in \Gamma_+^C$ only involves the values of $u(y,v)$ with $|x-y| < C\sqrt{L}$ and can be approximated by Taylor expansion when u is sufficiently regular.

Consider a point $x \in \Sigma$. The curvature of the circle is R^{-1}, and in some coordinate system, $x = (0, -R)$. The surfaces Σ^I and Σ^E are then the circles of center 0 and radius $R - lL$ and $R + lL$, respectively. We want to compute $\mathcal{R}^c u(x^I, \phi)$ for $\sin\phi \geq 0$. The contribution on Σ^I of the operator K in (4.11) is then given by

$$K^I u(x^E) = J(x^I)\frac{1}{2\pi}\int_0^\pi \sin\phi\frac{1}{\varepsilon}\Big(e^{-\sigma_a^c t(x^I,\phi)}u(\bar{x}(x^I,\phi)) - u(x^E)\Big)d\phi, \tag{4.23}$$

since $u(x^I) = u(x^E)$. We check that $J(x^I) = 1 + 2lL/(R-lL) = 1 + O(L)$.

We can represent any point $x = (x_1, x_2)$ on Σ^E in the vicinity of x^E by the angle ψ such that $\cos\psi = x_2/(R+lL)$ and $\sin\psi = x_1/R$. The distance between x and x^E on Σ^E is then given by $s(x) = (R+lL)\psi$. Notice that $s(x^E) = 0$. Also, any function $u(x)$ defined on Σ^E is a function in the coordinate s: $u(s(x)) \equiv u(x)$. Since $\bar{x}(x,\phi)$ and x^E belong to Σ^E, we have for u sufficiently regular that

$$u(\bar{x}(x^I,\phi)) = u(x^E) + s(\phi)\frac{\partial u(x^E)}{\partial s} + \frac{s^2(\phi)}{2}\frac{\partial^2 u(x^E)}{\partial s^2} + O(s^3(\phi)), \tag{4.24}$$

where we use $s(\phi) = s(\bar{x}(x^I,\phi))$. From the equation $\cos\psi = x^E \cdot \bar{x}(x^I,\phi)/(R+lL)^2$, we obtain that

$$s^2(\phi) = (R+lL)^2\psi^2 \approx 2(R+lL)(2lL - t\sin\phi). \tag{4.25}$$

with an error on s^2 of order L^2.

On the other hand, since t is small, we have $e^{-\sigma_a^c t} = 1 - \sigma_a^c t + O((\sigma_a^c t)^2)$. Using this expansion and (4.24) in (4.23), we observe that

$$\begin{aligned} K^I u(x^E) &= \frac{1}{\pi}\int_0^{\pi/2} \sin\phi\frac{1}{\varepsilon}\Big(-\sigma_a^c t(\phi)u(x^E) + \frac{s^2(\phi)}{2}\frac{\partial^2 u(x^E)}{\partial s^2}\Big)d\phi + \ldots \\ &\approx d^I\frac{\partial^2 u(x^E)}{\partial s^2} - \sigma_a^I u(x^E). \end{aligned} \tag{4.26}$$

since $s(\pi - \phi) = -s(\phi)$ and $t(\pi - \phi) = t(\phi)$. The higher order terms are at most of order $O(\varepsilon^{-1}[\sigma_a^c ts^2 + (\sigma_a^c t)^2 + s^4])$. We can show that the contribution $K^E u(x^E)$ (such that $K = K^I + K^E$ in (4.11)) has the same expression as $K^I u(x^E)$ at the leading order (we omit the tedious details). We see that up to higher order terms, the operator K in (4.11) is negative since $d^I > 0$ and $\sigma_a^I > 0$. Let us mention that for higher space dimensions and more complicated surfaces Σ, the operator $\frac{\partial^2}{\partial s^2}$ has to be replaced by the Laplace-Beltrami operator $\Delta_\perp$ on Σ^E.

It remains to find the scaling of L and σ_a^c such that d^I and σ_a^I are of order $O(1)$. (This scaling is actually independent of the spatial dimension n.) We therefore need to integrate $\sin\phi t(\phi)$ and $\sin\phi s^2(\phi)$ over $(0,\pi/2)$. Using the expansion in (4.22), the bound $t < C\sqrt{L}$, and $\phi_0 = \sqrt{L}$, we obtain that

$$\frac{1}{\pi}\Big(\int_0^{\phi_0} + \int_{\phi_0}^{\pi/2}\Big)\sin\phi t(\phi)d\phi = (R-lL)\frac{\tau}{4} + O(L^{3/2}) = lL + O(L^{3/2}).$$

Using (4.25) and (4.22), we obtain that

$$s^2(\phi)\sin\phi = \frac{4l^2L^2}{\sin\phi} + O(\frac{L^3}{\sin^3\phi}) + O(L^2).$$

On the other hand, we have that $s(\phi) < C\sqrt{L}$ independent of ϕ. Defining then again $\phi_0 = \sqrt{L}$, we obtain

$$\frac{1}{\pi}\Big(\int_0^{\phi_0} + \int_{\phi_0}^{\pi/2}\Big)\sin\phi s^2(\phi)d\phi = O(L^2|\ln\phi_0|) + O(\frac{L^3}{\theta_0^2}) + O(L^2) = O(L^2|\ln L|).$$

The above calculations allow us to obtain the following result:

Assume that the layer scales as

$$L^2|\ln L| = \varepsilon, \tag{4.27}$$

and that the absorption coefficient scales as

$$\sigma_a^c = \frac{L}{\varepsilon}\overline{\sigma}_a^c, \tag{4.28}$$

where $\overline{\sigma}_a^c$ is independent of ε. Then the operators K^I in (4.26) and K in (4.11) are of order 1. *Moreover, the approximation in (4.26) is found to be of order $L \approx \sqrt{\varepsilon}$ if we neglect the term* $|\ln L|$.

Indeed, the error terms in (4.26) are respectively of order L^2, ε, and the integral of $\varepsilon^{-1}\sin\phi s^4(\phi)$, of order $\varepsilon^{-1}L^4/\phi_0^2 = O(\varepsilon^{-1}L^3) \approx \sqrt{\varepsilon}$. Let us make two observations. First, the above scaling is the unique one that renders the correction $\mathcal{R}_1^c$ of order $O(1)$ when applied to functions that only depend on the spatial variable x. Second, the non-local operator K in (4.11) can actually be approximated by a *local* operator $2K^I$ as shown in (4.26). The accuracy of this local operator is however *only* of order $\sqrt{\varepsilon}$, whereas the theory predicts a difference between the transport solution and the generalized diffusion of order ε.

4.3. Straight Clear Layers. We now consider the case of straight clear layers. We still assume that $n = 2$ to simplify and define the clear layer Ω^C as

$$\Omega^C = \{x \in \Omega,\ |x_2| < lL\}. \tag{4.29}$$

For straight clear layers, as for curved layers, the critical size L that triggers order one modifications of the diffusion jump conditions is also given by (4.27) and (4.28).

This result could be obtained by letting $R \to \infty$ in the previous subsection. The derivation however is slightly different mainly because the travel time $t(x,\phi)$ is no longer bounded.

Let $x \in \Sigma = \Omega \cap \{x_2 = 0\}$ and x^I on Σ^I. The layer thickness is $2lL$. The traveling time $t(x^I,\phi) = 2lL/\sin\phi$. Therefore, we have

$$\mathcal{R}^c u(x^I,\phi) = u(x^E - \frac{2L\cos\phi}{\sin\phi},\phi) e^{-\sigma_a^c t(x^I,\phi)}.$$

Thanks to the results of the preceding section, we assume that the scaling of the absorption coefficient is $\sigma_a^c = L^{-1}\overline{\sigma}_a^c\varepsilon$, and obtain that the contribution to the operator K coming from the absorption term is $-2\sigma_a^I u(x^E)$.

The other contributions in the operator K take the form

$$A = \frac{1}{\varepsilon 2\pi}\int_0^\pi \sin\phi\Big(u(x^E - \frac{2lL\cos\phi}{\sin\phi}) - u(x^E)\Big)d\phi.$$

The integration over the subset ϕ or $\pi-\phi$ less than ϕ_0 gives a contribution of order $\varepsilon^{-1}\int_0^{\phi_0}\sin\phi d\phi = O(L^2/\varepsilon)$. And for $\phi_0 < \phi < \pi - \phi_0$, we observe that $2L/\sin\phi$ is small. Therefore, we obtain

$$u(x^E - \frac{2lL\cos\phi}{\sin\phi}) = u(x^E) - \frac{2lL\cos\phi}{\sin\phi}\partial_1 u(x^E) + \frac{2l^2L^2\cos^2\phi}{\sin^2\phi}\partial_{11}u(x^E) + \dots.$$

Again, the term involving the first-order derivative averages to 0 and we are left with

$$\int_{\phi_0}^{\pi-\phi_0}\frac{2l^2L^2\cos^2\phi}{\sin\phi}d\phi = O(L^2|\ln L|).$$

The main difference with the case of curved layers is that higher order terms are also of order $L^2 << L^2|\ln L|$. We again obtain that the integral operator K converges to the differential operator $2K^I$ given by the second line of (4.26) when $L^2|\ln L| = \varepsilon$, as in the case of curved clear layers. One might have expected that straight clear layers would trigger order-one modifications of the transport solution for smaller thicknesses than in the curved case because particles can travel longer inside the clear layer. The above analysis shows that most of the non-local effects generated by the clear layers are 'local' enough so that the difference of geometry between the two cases plays no significant role.

Notice to conclude this section that when we replace K by $2K^I$ given by the second line of (4.26), we neglect terms of order $L^2/\varepsilon = |\ln L|^{-1}$ that are truly non-local ($u(x^E - 2lL\cos\phi/\sin\phi)$ can be very different from $u(x^E)$ when ϕ is small). Therefore, the local operator $2K^I$ is a relatively crude approximation of K. For this reason, the numerical application of the following section uses the non local interface condition of (4.9) and the corresponding variational formulation (4.19)-(4.20), which, in the case of straight clear layers, substantially simplifies since $J \equiv 1$. Nonetheless, in both cases, the operator K converges to the local operator $2K^I$, which is a diffusion in the orthogonal directions to the direction of smaller thickness. The clear layer acts then as a *wave guide* along which photons can *diffuse*.

5. Numerical Application in the case of Straight Clear Layers. This section provides some numerical evidence that the solution to the modified diffusion equation (4.9)-(4.11) is an accurate approximation of the solution to the transport equation (4.2).

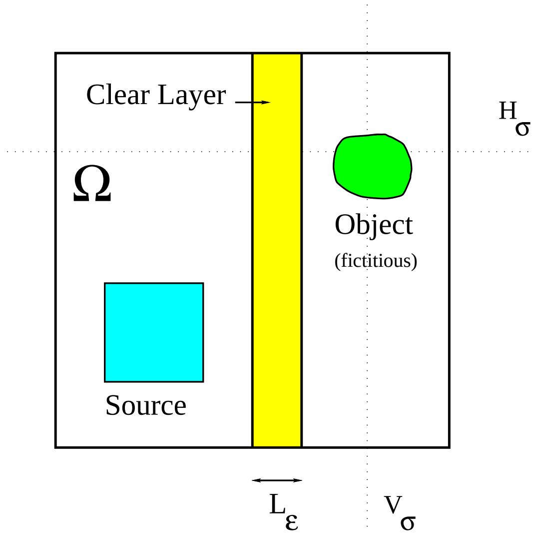

FIG. 5.1. *Geometry of the problem. The domain is diffusive except within the clear layer. The source is on one side of the layer and the region of interest (fictitious object) on the other side.*

To minimize the computational cost, the geometry considered here is a two-dimensional diffusive square surrounded by a vacuum and perforated throughout by a straight clear layer. A source of particles or energy density is present on one side of the clear layer. The numerical experiment considers a volume source (see Fig. 5.1). Non-vanishing incoming boundary conditions would give similar results. In practice, it is crucial to accurately predict the amount of energy reaching the object to be detected prior to using any inversion algorithm. In general, the objects to be detected, like tumors in diffuse tomography, and the sources of energy are on opposite sides of the clear layer [15]. The main goal is thus to show that the method presented in the previous section is capable of accurately predicting the particle density on the side of the clear layer where the objects are.

The square Ω, normalized to $(0,1)^2$, is discretized by a uniform grid composed of $N_x \times N_x$ identical meshes with $N_x = 120$. The velocity space, here the unit circle S^1, is discretized by $N_a = 96$ uniformly distributed directions. The mean free path is chosen to be $1/100$, which makes the domain Ω optically quite thick. The domain is non-absorbing. The size of the clear layer is $L = 0.1$. Notice that it is large compared with the mean free path, but still relatively small compared with the size of the domain. The clear layer is non-scattering and non-absorbing. So particles at one side of the layer travel through the layer along straight lines until they reach the opposite side or the boundary of the domain Ω. In relation with the theory of the preceding section, we have $\varepsilon = 0.01$ and $L = \sqrt{\varepsilon}$. Therefore, we can expect that the presence of the clear layer will significantly modify the transport solution.

The spatial discretization of the transport equation is diamond discretization [22], which is widely used in linear transport theory for its relative simplicity and second order accuracy. The diffusion equation is solved by the method of continuous finite elements of degree less than or equal to one both in x and y (Q_1 elements) [12]. The same finite elements are also used to accelerate the source iteration of the transport equation with satisfactory results (we refer to [19, 22] for the details on the source iteration method to solve the transport equation and its preconditioning by diffusion).

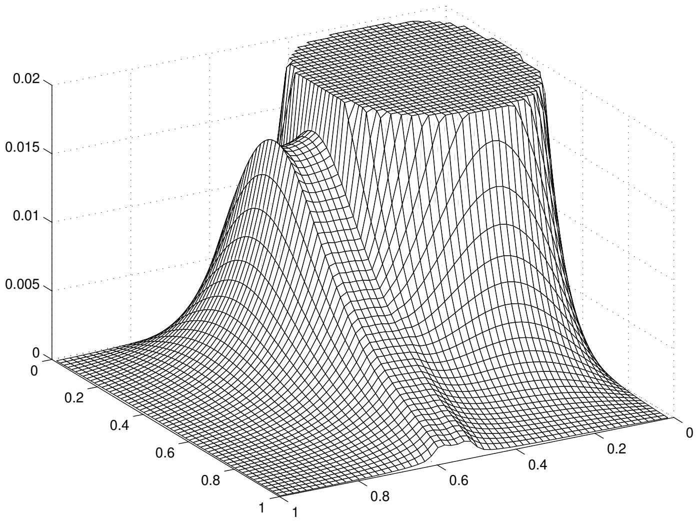

FIG. 5.2. *Solution of the transport equation seen from behind. The closest point to the viewer is the upper right edge, of coordinates* $(1, 1)$. *The solution has been truncated to display the density distribution in the vicinity of the layer.*

The source distribution is equal to 1 in the rectangle $(1/6, 7/24) \times (5/24, 9/24)$ and 0 outside. The solution of the transport problem in the vicinity of the clear layer is represented in Fig. 5.2. The solution has been truncated to 0.02 to display the effect induced by the clear layer (the maximum distribution is approximatively 0.8 and is attained inside the source region). Because of the clear layer, the density of particles coming from the source location and propagating along the clear layer is large enough to generate the channel-type flow observable within the layer.

We now test various diffusion models at our disposal and compare them to the transport solution. Four diffusion models are considered. The first one is the diffusion solution to (4.9)-(4.11) analyzed in this paper. It will be referred to as ASM, for *asymptotic model*. We also consider three other 'classical' diffusion models. The first one treats the clear layer as if it were diffusive. It is referred to as EDM, for *everywhere diffusive model*. This model simply consists in extending the validity of the diffusion approximation in the non-diffusive regions. The last two methods are essentially based on the opposite idea that since the clear layer is thin, it can be neglected. The NLM method (for *no layer model*) assumes that the whole domain is diffusive (with constant mean free path 1/100) as if the layer did not exist. The last method, CJC (for *classical continuity jump conditions*), treats the layer as an infinitesimally small interface, hence imposes continuity of flux and current across the interface (that is to say (4.9) with $K \equiv 0$).

As a general conclusion, we observe that ASM is fairly close to the transport solution, whereas the other models do not capture the salient characteristics of the clear layer. Fig. 5.3 compares the different diffusion approximations of the transport equation along the horizontal cross section H_σ shown in Fig. 5.1. We deduce that all diffusion theories except ASM give erroneous results.

In EDM, the non-scattering clear layer is represented by an infinite diffusion coefficient (taken large is the numerical simulation), whose effect is to instantly diffuse any particle reaching the clear layer uniformly along the boundaries of the clear layer.

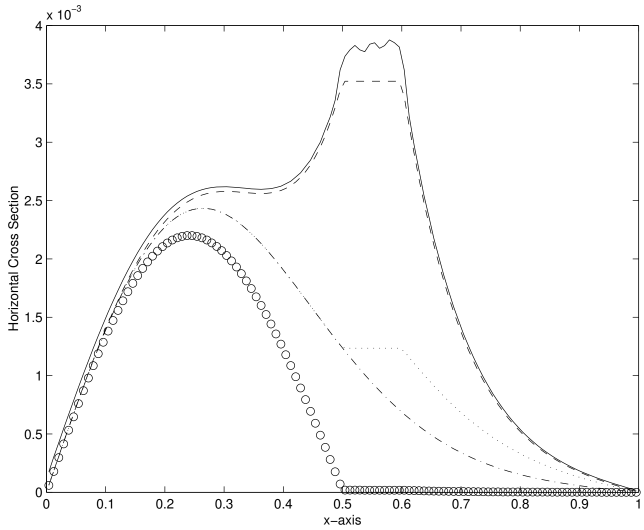

FIG. 5.3. *Horizontal cross section along H_σ of the velocity average of the transport solution (solid line) and different diffusion approximations: asymptotic model ASM (dashed line), diffusion approximation in the whole domain EDM (circles), diffusion approximation as if the clear layer was diffusive NLM (dash-dotted line), and diffusion approximation with continuity of the solution and its current across the interface CJC (dotted line). The cross section H_σ has for vertical coordinate* $y = 0.8$.

Hence, the diffusion approximation behaves as if the layer were very large. Because of the geometry of Ω, the distribution reaches a value close to 0 at the boundary of the clear layer and almost no particles can cross the clear layer. This is confirmed by the circles in Fig. 5.3. Treating the clear layer as a diffusive object is the worst possible choice in this configuration. More generally, EDM will always overestimate the dispersiveness of the clear layer, even for thin clear layers with large, but not infinite, diffusion coefficient. This is consistent with the numerical simulations in [17].

The NLM method (dash-dotted line) is clearly valid for clear layers that are too thin to trigger any significant effect on the transport solution. Fig. 5.3 however shows that it does not account for the dispersiveness of thick enough clear layers. The CJC method, shown in dotted line, accounts for the geometry of the layer better than NLM, but clearly misses the dispersive effects as well.

ASM, represented in dashed line in Fig. 5.3, perfectly measures the dispersiveness of the clear layer. Except within the clear layer, the agreement between the two curves is visually almost perfect. The discrepancy inside the clear layer may show the limitations of the approximation, where the outgoing flow of particles at the boundary of Ω is not accounted for. Notice that the agreement in the region on the right of the layer is still visually almost perfect.

Other horizontal cross sections would yield similar conclusions. This is confirmed by the results shown in Fig. 5.4, where the same solutions as above are represented along the cross section V_σ (see Fig. 5.1). As already mentioned, treating the clear layer as a diffusive object (EDM) prevents particles from crossing the layer and the solution of the right side of the layer almost vanishes (circles). In the vicinity of the source (for $y \approx 0.3$ in the figure), the density of particles is less important when a clear layer is present since particles can travel along the transverse direction. Therefore,

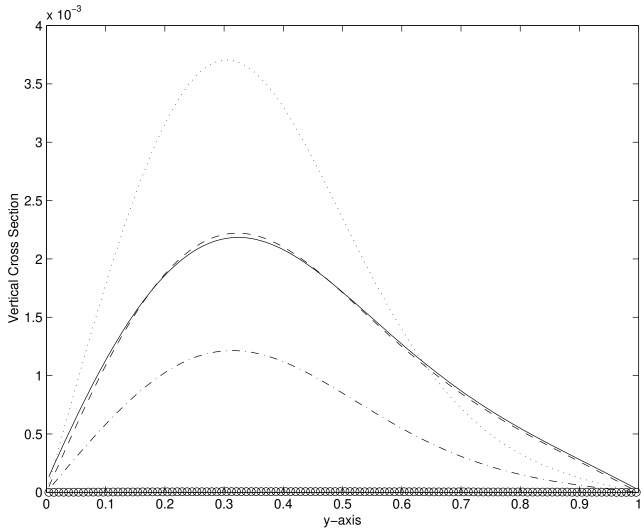

FIG. 5.4. *Same as Fig. 5.3 for the vertical cross section along V_σ, of horizontal coordinate* $x = 0.8$.

CJC, imposing continuity of current across the clear layer, is an upper bound to the exact solution in this area. However, in those areas where the density is small in the absence of clear layer because of geometrical spreading, but large when the clear layer is present because of its dispersiveness, CJC provides a lower bound of the exact solution. This is confirmed by the behavior of the dotted curve in Fig. 5.4. The dashed-dotted curve shows that diffusive spreading exceeds the dispersive behavior of the clear layer since the NLM solution remains below the exact solution along the whole cross section V_σ. Notice that the asymptotic model ASM again provides a very accurate description of the transport solution.

We now consider some quantitative data on the accuracy of the diffusion approximations. One of the main objectives is to obtain an accurate description of the photon density on the right side of the clear layer. To this purpose, we introduce

$$e_m(x) = \frac{\displaystyle\int_V u(x,v)d\mu(v) \; - u_m(x)}{\displaystyle\int_V u(x,v)d\mu(v)}, \tag{5.1}$$

where u_m is the diffusion solution of a model m and e_m the corresponding relative error. We also denote by $\Omega_1 = (0.6, 0.9) \times (0.1, 0.9)$ the subset of Ω on the right side of the clear layer that excludes a small strip in the vicinity of the boundary of the domain, where the error e_m becomes large because of the Dirichlet conditions imposed to the diffusion models. Table 5.1 shows the $L^2(\Omega_1)$-norm of the relative error e_m for the different models. These results corroborate those of Fig. 5.3 and Fig. 5.4 and validate for this experiment the jump conditions of the asymptotic model (4.9)-(4.11).

Acknowledgment. This work was supported in part by NSF Grant DMS-0072008.

REFERENCES

TABLE 5.1
$L^2(\Omega_1)$-norm of the relative errors e_m for different models. $|\Omega_1|$ stands for the volume of the domain Ω_1.

Model:	ASM	NLM	EDM	CJC
$\dfrac{\Vert e_m\Vert_{L^2(\Omega_1)}}{\vert\Omega_1\vert}$	0.0289	0.9967	0.5228	0.5712

[1] R. A. ADAMS, *Sobolev Spaces*, Academic Press, NY, San Francisco, London, 1975.

[2] G. ALLAIRE AND G. BAL, *Homogenization of the criticality spectral equation in neutron transport*, M2AN Math. Model. Numer. Anal., 33 (1999), pp. 721–746.

[3] S. R. ARRIDGE, *Optical tomography in medical imaging*, Inverse Problems, 15 (1999), pp. R41–R93.

[4] S. R. ARRIDGE AND J. C. HEBDEN, *Optical Imaging in Medicine: II. Modelling and reconstruction*, Phys. Med. Biol., 42 (1997), pp. 841–853.

[5] G. BAL, *Boundary layer analysis in the homogenization of neutron transport equations in a cubic domain*, Asymptot. Anal., 20(3-4) (1999), pp. 213–239.

[6] G. BAL AND L. RYZHIK, *Diffusion Approximation of Radiative Transfer Problems with Interfaces*, SIAM J.Appl. Math., 60(6) (2000), pp. 1887–1912.

[7] G. BAL AND X. WARIN, *Discrete Ordinates Methods in xy-Geometry with spatially varying angular discretization*, *Nuclear Science and Engineering*, 127(2) (1997), pp. 169–181.

[8] C. BARDOS, R. SANTOS, AND R. SENTIS, *Diffusion approximation and computation of the critical size*, Trans. Am. Math. Soc., 284 (1984), pp. 617–649.

[9] A. BENSOUSSAN, J.-L. LIONS, AND G. PAPANICOLAOU, *Boundary layers and homogenization of transport processes*, Res. Inst. Math. Sci., Kyoto Univ., 15 (1979), pp. 53–157.

[10] K. M. CASE AND P. F. ZWEIFEL, *Linear Transport Theory*, Addison-Wesley series in nuclear engineering, Addison-Wesley, Reading, Mass., 1967.

[11] S. CHANDRASEKHAR, *Radiative Transfer*, Dover Publications, New York, 1960.

[12] P. G. CIARLET, *The finite element method for elliptic problems*, North-Holland, 1978.

[13] R. DAUTRAY AND J.-L. LIONS, *Mathematical Analysis and Numerical Methods for Science and Technology. Vol.6*, Springer Verlag, Berlin, 1993.

[14] J. J. DUDERSTADT AND W. R. MARTIN, *Transport Theory*, Wiley-Interscience, New York, 1979.

[15] M. FIRBANK, S. A. ARRIDGE, M. SCHWEIGER, AND D. T. DELPY, *An investigation of light transport through scattering bodies with non-scattering regions*, Phys. Med. Biol., 41 (1996), pp. 767–783.

[16] F. GOLSE, S. JIN, AND C. D. LEVERMORE, *The convergence of numerical transfer schemes in diffusive regimes. I. Discrete-ordinate method.*, SIAM J. Numer. Anal., 36 (1999), pp. 1333–1369.

[17] A. H. HIELSCHER, R. E. ALCOUFFE, AND R. L. BARBOUR, *Comparison of finite-difference transport and diffusion calculations for photon migration in homogeneous and heterogeneous tissues*, Phys. Med. Biol., 43 (1998), pp. 1285–1302.

[18] A. ISHIMARU, *Wave Propagation and Scattering in Random Media*, New York: Academics, 1978.

[19] E. W. LARSEN, *Unconditionally Stable Diffusion-Acceleration of the Transport Equation*, Transport Theory Statist. Phys., 11 (1982), pp. 29–52.

[20] E. W. LARSEN AND J. B. KELLER, *Asymptotic solution of neutron transport problems for small mean free paths*, J. Math. Phys., 15 (1974), pp. 75–81.

[21] E. W. LARSEN, J. E. MOREL, AND W. F. MILLER JR., *Asymptotic solutions of numerical transport problems in optically thick, diffusive regimes*, J. Comp. Phys., 69 (1987), p. 283.

[22] E. E. LEWIS AND W. F. MILLER JR., *Computational Methods of Neutron Transport*, J. Wiley and sons, New York, 1984.

[23] J. M. LUCK AND T. M. NIEUWENHUIZEN, *Light Scattering from Mesoscopic Objects in Diffusive Media*, Eur. Phys. J. B, 7(3) (1999), pp. 483–500.

[24] L. RYZHIK, G. PAPANICOLAOU, AND J. B. KELLER, *Transport equations for elastic and other waves in random media*, Wave Motion, 24 (1996), pp. 327–370.

[25] H. SATO AND M. C. FEHLER, *Seismic wave propagation and scattering in the heterogeneous earth*, AIP series in modern acoustics and signal processing, AIP Press, Springer, New York, 1998.

[26] M. VAN ROSSUM AND T. NIEUWENHUIZEN, *Multiple scattering of classical waves: microscopy, mesoscopy, and diffusion*, Rev. Modern Phys., 71(1) (1999), pp. 313–371.