Lecture 10
Derivation of the Diffusion Equation

In this lecture, we give two very different techniques for deriving the diffusion equation. The first is based upon a Galerkin method in angle, and the second is based upon an asymptotic expansion.

1 A Galerkin Method

We begin with the differential transport equation:

$$\mu\frac{\partial\psi}{\partial x} + \sigma_t\psi = \frac{\sigma_s}{4\pi}\,\phi + \frac{Q_o}{4\pi}\,. \tag{1}$$

We propose a Galerkin approximation to Eq. (1) based upon a linear trial space of the following form:

$$\psi(x,\mu) = \frac{a(x)}{4\pi} + \frac{3b(x)\mu}{4\pi}\,, \tag{2}$$

with the weighting space equal to the trial space. Note that

$$2\pi\int_{-1}^{+1}\psi(x,\mu)\,d\mu = \phi(x) = a(x)\,, \tag{3a}$$

$$2\pi\int_{-1}^{+1}\psi(x,\mu)\mu\,d\mu = J(x) = b(x)\,. \tag{3b}$$

Thus Eq. (2) can be rewritten as

$$\psi(x,\mu) = \frac{\phi(x)}{4\pi} + \frac{3J(x)\mu}{4\pi}\,. \tag{4}$$

Substituting from Eq. (4) into Eq. (1) and integrating over all directions, we get the zero'th moment or balance equation:

$$\frac{\partial J}{\partial x} + \sigma_a = Q_0\,. \tag{5}$$

Substituting from (4) into (1) multiplying by μ, and integrating over all directions we get the the first-moment equation:

$$\frac{1}{3}\frac{\partial \phi}{\partial x} + \sigma_t J = 0\,. \tag{6}$$

Using Eq. (6) to solve for J, we get Fick's law:

$$J = -D\frac{\partial \phi}{\partial x}\,, \tag{7}$$

where

$$D = \frac{1}{3\sigma_t}\,. \tag{8}$$

Substituting from Eq. (7) into Eq. (5) we get the diffusion equation:

$$-\frac{\partial}{\partial x}D\frac{\partial \phi}{\partial x} + \sigma_a\phi = Q_0\,. \tag{9}$$

Thus we see from the derivation that the diffusion equation is exact whenever the flux is either isotropic or linearly anisotropic. However, the derivation gives no hint as to when one would expect the transport solution to be linear in angle. Furthermore, if the Galerkin approximation is made for the time-dependent transport equation rather than the steady-state equation, one does not obtain the diffusion equation unless one also assumes that $\frac{\partial J}{\partial t} = 0$.

1.1 Asymptotic Derivation

We next use asymptotics to obtain the time-dependent diffusion equation. Unlike the Galerkin derivation, this derivation does give insight into the conditions under which one would expect the transport solution to be linear in μ and hence diffusive. The central theme of our asymptotic expansion is to first use a "small" dimensionless parameter, ϵ, to scale parameters in a non-dimensional form of the transport equation, and thereby establish the relative sizes of these parameters in the limit as $\epsilon \to 0$. The transport solution is then expanded in a power series in ϵ, and substituted into the scaled transport equation. The terms of that equation that multiply each power of ϵ are grouped together to obtain a hierarchical system of equations for the solution. Our purpose here is to define an asymptotic expansion of the transport equation with a leading-order solution that satisfies the diffusion equation, thereby defining a formal mathematical limit in which transport theory becomes equivalent to diffusion theory.

We begin with the time-dependent transport equation:

$$\frac{1}{v}\frac{\partial\psi}{\partial t} + \mu\frac{\partial\psi}{\partial x} + \sigma_t\psi = \frac{\sigma_s}{4\pi}\phi + \frac{Q_0}{4\pi}\,. \tag{10}$$

The following quantities are defined as follows for the purpose of putting this equation in a non-dimensional form.

$\bar{\psi}$: a constant value of ψ that is characteristic of the solution for ψ.

Δt: a time scale characteristic of the solution for ψ is defined.

Δx: A spatial scale length characteristic of the solution for ψ.

The temporal and spatial scale lengths are used to define a non-dimensional time variable,

$$t' = \frac{t}{\Delta t}\,, \tag{11}$$

and a non-dimensional spatial variable,

$$x' = \frac{x}{\Delta x} \tag{12}$$

respectively. Finally, we obtain the desired non-dimensional form of the transport equation by dividing Eq. (10) by $\sigma_t\bar{\psi}$, transforming to the non-dimensional time and space variables, and expressing σ_s as $\sigma_t - \sigma_a$:

$$\alpha\frac{\partial\hat{\psi}}{\partial t'} + \beta\mu\frac{\partial\hat{\psi}}{\partial x'} + \hat{\psi} = (1-\gamma)\,\hat{\phi} + \hat{Q}_0\,, \tag{13}$$

where

$$\alpha = \frac{1}{\sigma_t v \Delta t}\,, \tag{14}$$

$$\hat{\psi} = \frac{\psi}{\bar{\psi}}\,, \tag{15}$$

$$\beta = \frac{1}{\sigma_t \Delta x}\,, \tag{16}$$

$$\hat{\phi} = \frac{\phi}{4\pi\bar{\psi}}\,, \tag{17}$$

$$\gamma = \frac{\sigma_a}{\sigma_t}\,, \tag{18}$$

$$\hat{Q}_0 = \frac{Q_0}{\sigma_t 4\pi\bar{\psi}}\,. \tag{19}$$

The parameter, α, represents the mean time between particle collisions divided by the time scale of the solution, the parameter, β, represents the mean-free-path divided by the spatial scale length of the solution, the parameter γ represents the probability that a particle undergoing an interaction will be absorbed, and the parameter $\hat{Q}_0$ represents the source rate divided by the characteristic total interaction rate. To determine the scalings that leads to the diffusion equation to leading order, we first express the diffusion equation in analogous dimensionless form:

$$\alpha\frac{\partial\hat{\phi}}{\partial t'} - \beta\frac{\partial}{\partial x'}\frac{\beta}{3}\frac{\partial\hat{\phi}}{\partial x'} + \gamma\hat{\phi} = \hat{Q}_0\,. \tag{20}$$

If the asymptotic expansion is to yield diffusion solution to leading order, the diffusion equation must be invariant to the scaling of the dimensionless parameters. The simplest acceptable scalings are obtained via multiplication of Eq. (20) by ϵ^2, which immediately yields:

$$\alpha \rightarrow \alpha\epsilon^2 \,, \tag{21}$$

$$\beta \rightarrow \beta\epsilon \,, \tag{22}$$

$$\gamma \rightarrow \gamma\epsilon^2 \,, \tag{23}$$

$$\hat{Q}_0 \rightarrow \hat{Q}_0\epsilon^2 \,. \tag{24}$$

These scalings imply that the asymptotic diffusion solution is associated with a mean time between collisions that is "very much smaller" than the characteristic time interval of the solution, a mean-free-path that is "much smaller" than the characteristic spatial dimension of the solution, an absorption cross section that is "very much smaller" than the total cross section, and a source rate that is "very much smaller" than the characteristic total interaction rate.

Applying these scalings to Eq. (13), we get

$$\epsilon^2\alpha\frac{\partial\hat{\psi}}{\partial t'} + \epsilon\beta\mu\frac{\partial\hat{\psi}}{\partial x'} + \hat{\psi} = \left(1 - \gamma\epsilon^2\right)\hat{\phi} + \hat{Q}_0\epsilon^2 \,. \tag{25}$$

The primary purpose of the non-dimensionalization is both to obtain a physical understanding of the scaling and to make sure that there are no inconsistencies in the scaling. Although one can perform the asymptotics on the non-dimensional equation and then convert the results back to dimensional form, we prefer to first convert the scaled non-dimensional equation to dimensional form and then perform the asymptotics. Thus we next express Eq. (25) in dimensional form:

$$\frac{\epsilon^2}{v}\frac{\partial\psi}{\partial t} + \epsilon\mu\frac{\partial\psi}{\partial x} + \sigma_t\hat{\psi} = \frac{\sigma_t - \sigma_a\epsilon^2}{4\pi}\phi + \frac{Q_0\epsilon^2}{4\pi}\,. \tag{26}$$

The solution to Eq. (26) is next expanded in powers of ϵ:

$$\psi(t,x,\mu) = \sum_{n=0}^{\infty}\psi^{(n)}(t,x,\mu)\,\epsilon^n\,. \tag{27}$$

Substituting from Eq. (27) into Eq. (26), we collect terms associated with each order of ϵ. The following equations are obtained.

The equation for order ϵ^0:

$$\psi^{(0)} = \frac{1}{4\pi}\phi^{(0)}\,. \tag{28}$$

This equation states that the leading order solution is isotropic in angle.

The equation for order ϵ^1:

$$\mu\frac{\partial\psi^{(0)}}{\partial x} + \sigma_t\psi^{(1)} = \frac{\sigma_t}{4\pi}\phi^{(1)}\,. \tag{29}$$

Integrating Eq. (29) over all directions, and recognizing that the integral of $\psi^{(1)}$ is $\phi^{(1)}$, we get what is called a solvability condition:

$$2\pi\int_{-1}^{+1}\mu\frac{\partial\psi^{(0)}}{\partial x}\,d\mu = 0\,. \tag{30}$$

Taking Eq. (28) into account, we find that Eq. (30) is indeed satisfied. Rearranging Eq. (29), and taking Eq. (28) into account, we get

$$\psi^{(1)} = \frac{1}{4\pi}\phi^{(1)} - \frac{\mu}{4\pi\sigma_t}\frac{\partial\phi^{(0)}}{\partial x} \,. \tag{31}$$

Equation (31) states that the first-order component of the solution is linearly anisotropic in μ. The equation for order ϵ^2:

$$\frac{1}{v}\frac{\partial\psi^{(0)}}{\partial t} + \mu\frac{\partial\psi^{(1)}}{\partial x} + \sigma_t\psi^{(2)} = \frac{\sigma_t}{4\pi}\phi^{(2)} - \frac{\sigma_a}{4\pi}\phi^{(0)} + \frac{1}{4\pi}\hat{Q}_0 \,. \tag{32}$$

Substituting from Eqs. (28) and (31) into Eq. (32), integrating over all directions, and recognizing that the integral of $\psi^{(2)}$ is $\phi^{(2)}$, we get

$$\frac{1}{v}\frac{\partial\phi^{(0)}}{\partial t} - \frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial\phi^{(0)}}{\partial x} + \sigma_a\phi^{(0)} = Q_0 \,. \tag{33}$$

Equation (33) states that the leading-order solution to the asymptotic expansion satisfies the diffusion equation. It is in this sense that the transport equation becomes equivalent to the diffusion equation in the asymptotic limit defined here.

The asymptotic expansion associated with the diffusion limit is necessarily valid only in regions several mean-free-paths from boundaries, material interfaces, and source discontinutities. Sufficiently rapid variations in cross-sections or sources can render the scale length assumptions associated with the expansion invalid. The transport solution can be diffusive at the boundaries of diffusive regions, depending upon the incident angular flux shape, but it more often is not. The region of transition from a non-diffusive transport solution to a diffusive solution is only a few mean-free-paths thick and the solution within it generally varies quite rapidly. Such a region is referred to as a boundary layer.

If we assume that $\bar{\psi}$, Δt, and Δx are all O(1), i.e., independent of ϵ, the following dimensional or physical scalings can be obtained from the non-dimensional scalings:

$$v \rightarrow \frac{v}{\epsilon}\,, \tag{34}$$

$$\sigma_t \rightarrow \frac{\sigma_t}{\epsilon}\,, \tag{35}$$

$$\sigma_a \rightarrow \sigma_a \epsilon\,, \tag{36}$$

$$\frac{Q_0}{4\pi} \rightarrow \frac{Q_0}{4\pi}\epsilon\,. \tag{37}$$

These scalings can be used to create a sequence of transport problems and associated solutions that converge to an ϵ-independent solution of the diffusion equation. In particular, to obtain such a sequence, one first defines an arbitrary transport problem. Then one performs the physical scaling given above for a sequence of decreasing ϵ values starting with $\epsilon = 1$. Each value of ϵ yields a different problem, with $\epsilon = 1$ corresponding to the original problem. The transport solutions for this sequence of problems will converge to an ϵ-independent solution of the diffusion equation in any region where the asymptotic expansion is valid. One can also substitute these physical scalings into the standard transport equation and perform an asymptotic expansion for the solution. The process of non-dimensionalizing, expanding, and re-dimensionalizing is completely equivalent to directly performing an asymptotic expansion for the standard transport solution with above physical scalings.

We have not considered an asymptotic boundary-layer analysis, which yields the boundary conditions satisfied by the asymptotic diffusion solution. Such an analysis is very complex and requires exact transport solutions. Thus we will not consider it in detail here. However, we will give some results of a boundary-layer analysis for a half-space problem in the diffusion limit with $x \in [0, \infty]$ and an incident flux at $x = 0$ defined by $f(u)$ for $\mu > 0$. In general, there is a boundary layer in this problem within a few mean-free-paths of $x = 0$ that smoothly transitions to a diffusion solution that is constant in space. The value of this constant leading-order diffusion-limit solution is given to within a few percent by

$$\phi = 2\pi \int_0^1 \left(3\mu^2 + 2\mu\right) f(\mu)\, d\mu\,. \tag{38}$$

We stress that this constant solution does not apply within the boundary layer. The best one can do is obtain diffusion boundary conditions that yield the correct diffusion solution away from boundary layers. The diffusion equation cannot describe the transport solution within boundary layers. If one applies the Marshak condition to this problem (see the next section), one obtains

$$\phi = 2\pi \int_0^1 4\mu f(\mu)\, d\mu\,, \tag{39}$$

i.e., $\phi = 4j_{in}$. Note that both of these expressions yield the same result for an isotropic flux, $f(\mu) = 1/\pi$. In particular, $\phi = 4.0$. When the incident flux is isotropic, there is no boundary layer to leading order. Otherwise, there is a boundary layer.

Finally, we note that further analysis indicates that the diffusion approximation is actually exact through O(ϵ), i.e., the error is O(ϵ^2). In particular, the O(1) and O(ϵ) scalar flux solutions respectively satisfy

$$\frac{1}{v}\frac{\partial \phi^{(0)}}{\partial t} - \frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial \phi^{(0)}}{\partial x} + \sigma_a \phi^{(0)} = Q_0\,, \tag{40}$$

and

$$\frac{1}{v}\frac{\partial \phi^{(1)}}{\partial t} - \frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial \phi^{(1)}}{\partial x} + \sigma_a \phi^{(1)} = 0\,, \tag{41}$$

while the O(1), O(ϵ) and O(ϵ^2) currents respectively satisfy

$$J^{(0)} = 0\,, \tag{42}$$

$$J^{(1)} = \frac{1}{3\sigma_t}\frac{\partial \phi^{(0)}}{\partial x}\,, \tag{43}$$

and

$$J^{(2)} = \frac{1}{3\sigma_t}\frac{\partial \phi^{(1)}}{\partial x}\,. \tag{44}$$

Using Eqs.(40) through (43), it is not difficult to obtain the following results:

$$\frac{1}{v}\frac{\partial\left(\phi^{(0)} + \phi^{(1)}\epsilon\right)}{\partial t} - \frac{\partial}{\partial x}\frac{1}{3\sigma_t}\frac{\partial\left(\phi^{(0)} + \phi^{(1)}\epsilon\right)}{\partial x} + \sigma_a\left(\phi^{(0)} + \phi^{(1)}\epsilon\right) = Q_0\,, \tag{45}$$

$$J^{(0)} + J^{(1)}\epsilon + J^{(2)}\epsilon^2 = -\frac{\epsilon}{3\sigma_t}\frac{\partial\left(\phi^{(0)} + \phi^{(1)}\epsilon\right)}{\partial x}\,. \tag{46}$$

Thus the diffusion approximation is correct through $O(\epsilon)$ for the scalar flux and correct through $O(\epsilon^2)$ for the current.

1.2 Diffusion Boundary Conditions

We now consider boundary conditions based upon the Galerkin approximation for diffusion. Vacuum boundary conditions cannot be met exactly with our linear trial space. Thus we must meet them approximately. One of the most common approximations is the Marshak boundary condition. For instance, the exact vacuum boundary condition at $x = x_L$ is

$$\psi(x_L, \mu) = 0 \quad , \mu \geq 0, \tag{47}$$

The Marshak approximation to Eq. (9) preserves the rate of particle inflow:

$$2\pi \int_0^1 \psi(x_L, \mu)\mu \, d\mu = 0 \, . \tag{48}$$

Substituting from Eq. (4) into Eq. (48), and evaluating the integral, we get

$$\frac{\phi}{4} + \frac{J}{2} = 0 \, . \tag{49}$$

Using Eqs. (7) and (8), Eq. (49) can rewritten as

$$\phi - \left(\frac{2}{3} \lambda \frac{\partial \phi}{\partial x} \right) = 0 \, , \tag{50}$$

where $\lambda \equiv 1/\sigma_t$ is the mean-free-path. Equation (50) shows that the Marshak vacuum condition is equivalent to making the flux extrapolate to zero at a distance of 2/3 of a mean-free-path from the boundary, as illustrated in Fig. 1.

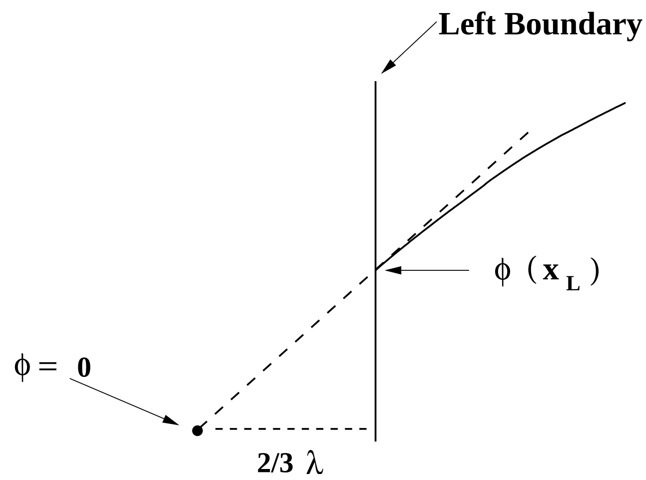

Figure 1: Solution extrapolation at boundary with vacuum condition.

Let us suppose that we have a non-zero angular flux, $f(\mu)$, incident at the left boundary. Then the exact boundary condition is the

$$\psi(x_L, \mu) = f(\mu) \quad , \mu \geq 0. \tag{51}$$

As in the vacuum case, the Marshak condition simply preserves the rate of particle inflow:

$$2\pi \int_0^1 \psi(x_L, \mu)\mu \, d\mu = 2\pi \int_0^1 f(\mu)\mu \, d\mu \,. \tag{52}$$

Substituting from Eq. (4) into Eq. (52), and evaluating the integral, we get

$$\frac{\phi}{4} + \frac{J}{2} = 2\pi \int_0^1 f(\mu)\mu \, d\mu \equiv j^+ \,, \tag{53}$$

where j^+ is called the half-range incoming current. Equation (53) can rewritten as

$$\phi - \left(\frac{2}{3}\lambda \frac{\partial \phi}{\partial x}\right) = 4j^+ \equiv \phi_b \,, \tag{54}$$

where $\frac{\phi_b}{4\pi}$ represents an "equivalent" isotropic boundary flux in the sense that $\frac{\phi_b}{4\pi}$ has the same incoming half-range current as $f(\mu)$. Thus we see from Eq. (54) that the Marshak

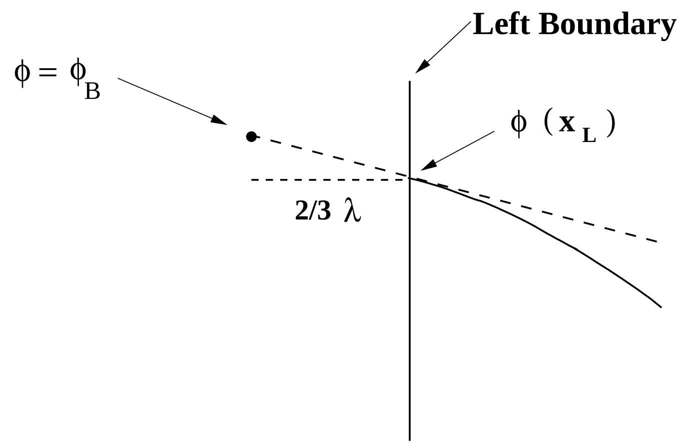

Figure 2: Solution extrapolation at boundary with source condition.

source condition is equivalent to making the scalar flux extrapolate to an equivalent boundary scalar flux value at a distance of 2/3 of a mean-free-path from the boundary. This is illustrated in Fig. 2.

A useful result from an asymptotic boundary layer analysis for a source condition is that a much more accurate extrapolated flux value can be computed as follows for anisotropic incident fluxes:

$$\phi_b \equiv 2\pi \int_0^1 f(\mu) \left(3\mu^2 + 2\mu\right) \, d\mu \,. \tag{55}$$

Note that this formula yields $\phi_b = 4j^+$ if the incident flux is isotropic. Furthermore, this formula can be used with any extrapolation distance.

Reflective (specular) boundary conditions must also be considered. Assuming such a condition at $x = x_L$, the exact transport boundary condition is

$$\psi(x_L, \mu) = \psi(x_L, -\mu) \quad , \mu \geq 0. \tag{56}$$

In this case, one simply sets $J = 0$ on the boundary. This is not unique to Marshak boundary conditions, but rather is the only physically correct choice.

Conditions at the interface between two dissimilar materials must also be considered. Let x_i denote the location of an interface. The transport angular flux solution must be continuous at a material interface. This implies that all angular moments of the angular flux must also be continuous. Thus the scalar flux and current must be continuous at a material interface. These are the interface conditions for the diffusion equation. As in the case of reflection, these conditions represent the only physically correct choice.

Marshak conditions are not the most accurate conditions for the diffusion equation, but they are the most accurate of the conditions that can be derived from simple physical considerations. More accurate conditions generally require information from exact transport solutions. For instance, asymptotic methods can be used to derive exact diffusion boundary conditions, but the associated boundary-layer analyses are very complicated and essentially require exact transport solutions.

We close this section by describing a technique for computing leakage rates that is independent of the extrapolation distance used and always conservative. We begin by making the following definitions for the half-range currents:

$$j^{+} = 2\pi \int_{0}^{1} \psi(\mu)\mu \, d\mu \,, \tag{57}$$

$$j^{-} = -2\pi \int_{-1}^{0} \psi(\mu)\mu \, d\mu \,. \tag{58}$$

Under these definitions, the net current is given by

$$J = j^{+} - j^{-} . \tag{59}$$

Because a diffusion solution satisfies the balance equation, balance will always be maintained if leakages are computed using Eq. (59). For instance, let us assume a source condition at the left boundary. Then the diffusion solution will yield J, and the correct physical value for j^{+} is known from the boundary condition. Thus using Eq. (59) to compute the leakage rate at the left boundary gives:

$$j^{-} = j^{+} - J . \tag{60}$$

This is the preferable practice whenever a non-Marshak boundary condition is used. When a Marshak boundary condition is used, Eq. (60) yields the same result as the direct use of Eq. (58).

2 An Example Diffusion Solution

We next solve the diffusion equation on $[0, x_0]$ with a constant isotropic distributed source, $\frac{Q_0}{4\pi}$, $\sigma_t = \sigma_s$, and vacuum boundary conditions. The equation to be solved is

$$-\frac{\partial}{\partial x} D \frac{\partial \phi}{\partial x} = Q_0 \quad , x \in [0, x_0], \tag{61}$$

with a left boundary condition given by

$$\frac{\phi}{4} + \frac{J}{2} = 0 \quad , x = 0, \tag{62a}$$

and a right boundary condition given by

$$-\frac{\phi}{4} + \frac{J}{2} = 0 \quad , x = x_0. \tag{62b}$$

The homogeneous solution to Eq. (61) is

$$\phi_h = a + bx\,, \tag{63}$$

and the particular solution is

$$\phi_p = -\frac{Q_0 x^2}{2D}\,. \tag{64}$$

Thus the total solution is

$$\phi = a + bx - \frac{Q_0 x^2}{2D}\,. \tag{65}$$

The constants a and b are determined by the boundary conditions. In particular, substituting from Eq. (65) into Eqs. (62a) and (62b), we respectively obtain

$$a - 2Db = 0\,, \tag{66a}$$

and

$$a + bx_0 - \frac{Q_0 x_0^2}{2D} = 2D\left(b - \frac{2Q_0 x_0}{2D}\right) = 0\,. \tag{66b}$$

Solving Eqs. (66a) and (66b), we get

$$a = Q_0 x_0 \,, \tag{67a}$$

$$b = \frac{Q_0 x_0}{2D} \,. \tag{67b}$$

Substituting from Eqs. (67a) and (67b) into Eq. (65), we obtain the following solution:

$$\phi = \frac{Q_0}{2D} \left(2D x_0 + x_0 x - x^2 \right) \,. \tag{68}$$