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Diffusion from a Point Source into a Space Bounded by an Impenetrable Plane

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DIFFUSION FROM A POINT SOURCE INTO A SPACE BOUNDED BY AN IMPENETRABLE PLANE

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§ 1. *Introduction*. The following mathematical model will be considered. In the cylindrical half-space $0 < r < \infty$, $0 < z < \infty$ particles of concentration $c(r, z)$ are subjected to a diffusion process determined by the constant D and to a mass transport parallel to the Z-axis with constant velocity $-w$. The plane $z = 0$ is a reflecting plane, i.e. the mass transport through that plane is zero. The particles are produced by a point source at the origin $z^2 + r^2 = 0$ of constant intensity Q.

The stationary state is determined by the partial differential equation

$$D\left(\frac{1}{r}\frac{\partial}{\partial r}\, r\,\frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial z^2}\right) + w\,\frac{\partial c}{\partial z} = 0, \tag{1.1}$$

the boundary condition

$$z = 0 \qquad \frac{\partial c}{\partial z} = 0, \tag{1.2}$$

and the condition of the point source (cf § 2)

$$z^2 + r^2 \to 0 \qquad c \sim \frac{Q}{2\pi D\sqrt{z^2 + r^2}}. \tag{1.3}$$

The model described above originated from an investigation by Boumans [1]) concerning the concentration of particles of a metal evaporated between two electrodes. The plane $z = 0$ corresponds to the lower electrode. If the unit of length is chosen in such a way that the unit circle $0 < r < 1$, $z = 0$ represents the surface of the lower electrode, the surface of the upper electrode is on the plane $z = 4$.

We quote the following values of D and w from an actual experiment: $D = 15\ \mathrm{cm}^2/\mathrm{s}$, $w = 720\ \mathrm{cm/s}$, radius of electrode surface 0.25 cm. Thus we may consider the following numerical example:

$$v = \frac{w}{2D} = 6.$$

The region which is of importance for the experiment is given by

$$0 \leq r \leq 1 \qquad 0 \leq z \leq 4.$$

Outside this region the model no longer represents the experimental conditions. Yet the model considered above may give a realistic picture if the concentration outside the region $0 \leq r \leq 1$, $0 \leq z \leq 4$ is very small compared to the concentration inside that region.

In fact we have found the result that for $v = 6$ only 0.166% of the total mass is outside the region considered. For $v = 3$ this figure becomes 4.45% and for $v = 2$ still only 13.5%.

§ 2. *Derivation of the solution.* The solution of (1.1) with diffusion from a point source of intensity Q at the origin with diffusion in the whole space $-\infty < z < \infty$ is well known, viz.

$$c_0(r, z) = \frac{Q}{4\pi D} \frac{e^{-v(z+\sqrt{z^2+r^2})}}{\sqrt{z^2 + r^2}}, \tag{2.1}$$

where $v = w/2D$. The meaning of the constant Q becomes apparent if we consider the mass transport through a small *sphere* of radius ϱ round the origin:

$$D \oint \frac{\partial c}{\partial n}\, \mathrm{d}\sigma = -\frac{Q}{4\pi} 4\pi\varrho^2 \frac{\partial}{\partial \varrho}\left(\frac{1}{\varrho}\right) = Q.$$

In a similar way the solution of (1.1) with diffusion in the half-space $0 < z < \infty$ behaves near the origin as given in (1.3). In the latter case we should consider the mass transport through a small *hemisphere* $\sqrt{z^2 + r^2} = \varrho$, $z > 0$ only:

$$D \oint \frac{\partial c}{\partial n}\, \mathrm{d}\sigma = -\frac{Q}{2\pi} 2\pi\varrho^2 \frac{\partial}{\partial \varrho}\left(\frac{1}{\varrho}\right) = Q.$$

The complete solution of (1.1) and (1.2) may be derived as follows.

We put

$$c(r,z) = \frac{Q}{2\pi D}\left[\frac{e^{-v(z+\sqrt{z^2+r^2})}}{\sqrt{z^2+r^2}} - \int\limits_{\infty}^{0} \varphi(\zeta)\,\frac{e^{-v(z-\zeta+\sqrt{(z-\zeta)^2+r^2})}}{\sqrt{(z-\zeta)^2+r^2}}\,d\zeta\right]. \quad (2.2)$$

Thus to twice the solution (2.1) for a point source we have added a continuum of point source solutions from sources at $z = -\zeta$, $r = 0$ with intensity $-2Q\varphi(\zeta)d\zeta$. The solution (2.2) clearly satisfies the differential equation (1.1). The unknown function $\varphi(\zeta)$ will be determined in such a way as to fulfil the boundary condition at $z = 0$.

If (2.2) is written as

$$c(r, z) = 2c_0(r, z) - \frac{Q}{2\pi D}\int\limits_{z}^{\infty} \varphi(z-t)\,\frac{e^{-v(t+\sqrt{t^2+r^2})}}{\sqrt{t^2+r^2}}\,dt,$$

the condition (1.2) gives

$$0 = \frac{-ve^{-vr}}{r} + \varphi(0)\,\frac{e^{-vr}}{r} - \int\limits_{z}^{\infty} \varphi'(-t)\,\frac{e^{-v(t+\sqrt{t^2+r^2})}}{\sqrt{t^2+r^2}}\,dt.$$

From this we obtain at once

$$\varphi(\zeta) = v.$$

Thus we have found the following solution

$$c(r, z) = 2c_0(r, z) - \frac{Qv}{2\pi D}\int\limits_{z}^{\infty} \frac{e^{-v(t+\sqrt{t^2+r^2})}}{\sqrt{t^2+r^2}}\,dt, \quad (2.3)$$

which in turn may be written as

$$c(r, z) = -\frac{Q}{2\pi D}\int\limits_{z}^{\infty} e^{-vt}\,d\,\frac{e^{-v\sqrt{t^2+r^2}}}{\sqrt{t^2+r^2}}. \quad (2.4)$$

The integral on the right-hand side of (2.3) may be reduced to the exponential integral

$$E_1(x) = -\,Ei(-x) = \int\limits_{x}^{\infty} \frac{e^{-t}}{t}\,dt. \quad (2.5)$$

We have

$$c(r, z) = \frac{Qv}{2\pi D}\left\{\frac{e^{-v(z+\sqrt{z^2+r^2})}}{v\sqrt{z^2+r^2}} - E_1\left[v(z+\sqrt{z^2+r^2})\right]\right\}. \quad (2.6)$$

The exponential integral may be expanded either for small x or for large x. We quote the following expansions

$$\mathrm{E}_1(x) = -\ln x - \gamma + x - \frac{x^2}{2!2} + \frac{x^3}{3!3} \cdots \qquad x > 0,$$

$$\mathrm{E}_1(x) \sim \frac{e^{-x}}{x}\left(1 - \frac{1!}{x} + \frac{2!}{x^2} - \frac{3!}{x^3} \cdots\right) \qquad x > 0.$$

§ 3. *Auxiliary expressions.* We shall derive an expression for the total concentration at the level z:

$$C(z) = 2\pi \int_0^\infty rc(r, z)\mathrm{d}r. \tag{3.1}$$

The function satisfies the differential equation

$$\frac{\mathrm{d}^2C}{\mathrm{d}z^2} + 2v\frac{\mathrm{d}C}{\mathrm{d}z} = 0,$$

which is obtained by integration of (1.1). Since $C \to 0$ for $z \to \infty$, $C(z)$ is of the form

$$C(z) = C(0)\, e^{-2vz}.$$

From (2.6) we obtain

$$C(0) = \frac{Q}{vD}\int_0^\infty \left(\frac{e^{-t}}{t} - \mathrm{E}_1(t)\right) t\,\mathrm{d}t = \frac{Q}{vD}\left[1 - \tfrac{1}{2}\int_0^\infty \mathrm{E}_1(t)\mathrm{d}t^2\right] =$$

$$= \frac{Q}{vD}\left[1 - \tfrac{1}{2}\int_0^\infty e^{-t}\,t\,\mathrm{d}t\right] = \frac{Q}{2vD} = \frac{Q}{w},$$

so that

$$C(z) = \frac{Q}{w}\, e^{-2vz}. \tag{3.2}$$

We may remark that the same expression is obtained if we start from the solution $c_0(r, z)$ of a point source of intensity Q diffusing into the whole space $-\infty < z < \infty$, $0 < r < \infty$.

Next we shall derive an expression for the total concentration at the level z outside the circle $r = R$:

$$A(R, z) = 2\pi \int_R^\infty rc(r, z)\mathrm{d}r. \tag{3.3}$$

From (2.4) we obtain

$$A(R, z) = -\frac{Q}{vD}\int_{z}^{\infty} e^{-vt}\, d\, e^{-v\sqrt{t^2+R^2}},$$

which may be brought into the form

$$A(R, z) = \frac{Q}{2D}\int_{z+\sqrt{z^2+R^2}}^{\infty} e^{-vu}\left(1 - \frac{R^2}{u^2}\right) du,$$

or finally

$$A(R, z) = \\ = \frac{Q}{w}\left\{\left(1 - \frac{vR^2}{z+\sqrt{z^2+R^2}}\right) e^{-v(z+\sqrt{z^2+R^2})} + v^2R^2 E_1[v(z+\sqrt{z^2+R^2})]\right\}. \quad (3.4)$$

In particular we have at $z = 0$

$$C(0) = \frac{Q}{w},$$

$$A(R, 0) = \frac{Q}{w}\{(1 - vR)e^{-vR} + v^2R^2E_1(vR)\}.$$

From the asymptotic expansion of $E_1(x)$ for $x \to \infty$ we obtain the following approximation for large vR:

$$A(R, 0) \sim \frac{Q}{w}\frac{2e^{-vR}}{vR}\left(1 - \frac{3}{vR} + \ldots\right).$$

We shall now determine the total mass outside the cylinder $0 < z < 4$, $0 < r < 1$ for the case $v = 6$. The total mass in $0 < z < \infty$, $0 < r < \infty$ is immediately obtained from (3.2):

$$M = \int_0^{\infty} C(z)dz = \frac{QD}{w^2}.$$

The total mass above the plane $z = 4$ is

$$M_1 = \int_4^{\infty} C(z)dz = \frac{QD}{w^2} e^{-8v},$$

which is entirely negligible. The total mass outside the cylinder $0 < z < \infty$, $0 < r < 1$ is

$$M_2 = \int_0^\infty A(1, z)\,\mathrm{d}z = \frac{Q}{2D}\int_0^\infty \mathrm{d}z \int_{z+\sqrt{z^2+1}}^\infty \mathrm{e}^{-vu}\left(1 - \frac{1}{u^2}\right)\mathrm{d}u =$$

$$= \frac{Q}{2D}\int_1^\infty \mathrm{e}^{-vu}\left(1 - \frac{1}{u^2}\right)\mathrm{d}u \int_0^{\frac{1}{2}\left(u-\frac{1}{u}\right)} \mathrm{d}z = \frac{QD}{w^2}\int_v^\infty \mathrm{e}^{-t}\left(1 - \frac{v^2}{t^2}\right)^2 t\,\mathrm{d}t =$$

$$= \frac{QD}{w^2}\left\{\left(1 + v + \frac{v^2}{2} - \frac{v^3}{2}\right)\mathrm{e}^{-v} + 2v^2\left(-1 + \frac{v^2}{4}\right)\mathrm{E}_1(v)\right\}.$$

The total mass outside the finite cylindrical region $0 < z < 4$, $0 < r < 1$ is less than $M_1 + M_2$. If $v = 6$, we have

$$\frac{w^2}{QD} M_1 = 1.4 \times 10^{-21}, \quad \frac{w^2}{QD} M_2 = 1.66 \times 10^{-3}.$$

Thus for $v = 6$ only 0.166% of the total mass is outside the region $0 < z < 4$, $0 < r < 1$. For $v = 3$ this figure is 4.45% and for $v = 2$ still 13.5%.

§ 4. *Appendix*. We mention the following alternative method which gives the solution in a different form. The partial differential equation (1.1) is satisfied by the elementary solution

$$\mathrm{J}_0(\lambda r)\mathrm{e}^{-z(v+\sqrt{\lambda^2+v^2})}, \tag{4.1}$$

λ being an arbitrary parameter. From this we may construct the general solution

$$c(r, z) = \int_0^\infty f(\lambda)\mathrm{J}_0(\lambda r)\mathrm{e}^{-z(v+\sqrt{\lambda^2+v^2})}\,\mathrm{d}\lambda. \tag{4.2}$$

In particular the point source solution $c_0(r, z)$ may be obtained in this way

$$\int_0^\infty \frac{\lambda}{\sqrt{\lambda^2 + v^2}}\mathrm{J}_0(\lambda r)\mathrm{e}^{-z(v+\sqrt{\lambda^2+v^2})}\,\mathrm{d}\lambda = \frac{\mathrm{e}^{-v(z+\sqrt{z^2+r^2})}}{\sqrt{z^2 + r^2}}. \tag{4.3}$$

Formula (4.3) may be derived from the following Laplace transform (cf. Erdélyi, Integral transforms I, 4.15.9)

$$\int_b^\infty e^{-pt} J_0(a\sqrt{t^2 - b^2})\, dt = \frac{e^{-b\sqrt{p^2+a^2}}}{\sqrt{p^2 + a^2}}. \tag{4.4}$$

In view of the condition (1.3) the function $f(\lambda)$ may be written as

$$f(\lambda) = \frac{Q}{2\pi D}\left[\frac{\lambda}{\sqrt{\lambda^2 + v^2}} - \psi(\lambda)\right], \tag{4.5}$$

where $\psi(\lambda) \to 0$ for $\lambda \to \infty$. From the condition (1.2) we obtain

$$\int_0^\infty (v + \sqrt{\lambda^2 + v^2})\psi(\lambda) J_0(\lambda r) d\lambda = \frac{v e^{-vr}}{r}.$$

From Erdélyi Integral transforms II, 8.2.4 we quote the following Hankel transform:

$$\int_0^\infty \frac{x}{\sqrt{a^2 + x^2}} J_0(xy) dx = \frac{e^{-ay}}{y}. \tag{4.6}$$

Thus we have

$$\psi(\lambda) = \frac{\lambda}{\sqrt{\lambda^2 + v^2}} \frac{v}{v + \sqrt{\lambda^2 + v^2}}.$$

Substitution of this expression into (4.4) and (4.2) gives

$$c(r, z) = \frac{Q}{2\pi D}\int_0^\infty \frac{\lambda}{v+\sqrt{\lambda^2+v^2}} J_0(\lambda r) e^{-z(v+\sqrt{\lambda^2+v^2})}\, d\lambda. \tag{4.7}$$

It is possible to reduce this expression to the form (2.3) or (2.4). We have

$$c(r, z) = \frac{Q}{2\pi D}\int_z^\infty e^{-vt}\, dt \int_0^\infty \lambda J_0(\lambda r) e^{-t\sqrt{\lambda^2+v^2}}\, d\lambda =$$

$$= \frac{Q}{2\pi D}\int_z^\infty e^{-vt}\, dt \int_v^\infty u J_0(r\sqrt{u^2 - v^2})\, e^{-ut}\, du =$$

$$= -\frac{Q}{2\pi D}\int_{z}^{\infty} \mathrm{e}^{-vt}\,\mathrm{d}\left[\int_{v}^{\infty} \mathrm{J}_0(r\sqrt{u^2 - v^2})\,\mathrm{e}^{-ut}\,\mathrm{d}u\right] =$$

$$= -\frac{Q}{2\pi D}\int_{z}^{\infty} \mathrm{e}^{-vt}\,\mathrm{d}\,\frac{\mathrm{e}^{-v\sqrt{t^2+r^2}}}{\sqrt{t^2 + r^2}},$$

where in the last line again (4.4) has been applied.

§ 5. *Generalization.* In a similar way the solution may be found of the diffusion equation in the region $z > 0$, $0 < r < \infty$:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c}{\partial r}\right) + \frac{\partial^2 c}{\partial z^2} + 2v\frac{\partial c}{\partial z} = 0, \tag{5.1}$$

with a reflecting plane

$$z = 0, \quad \frac{\partial c}{\partial z} = 0, \tag{5.2}$$

and a point source at $z = a$, $r = 0$.

The solution is

$$c(r,z) = c_0(r, z-a) + \mathrm{e}^{2av}c_0(r, z+a) - \frac{Qv}{2\pi D}\,\mathrm{e}^{2av}\int_{z+a}^{\infty}\frac{\mathrm{e}^{-v(t+\sqrt{t^2+r^2})}}{\sqrt{t^2+r^2}}\,\mathrm{d}t, \tag{5.3}$$

or

$$c(r,z) = c_0(r,z-a) + \mathrm{e}^{2av}c_0(r,z+a) - \frac{Qv}{2\pi D}\,\mathrm{E}_1[v(z+a+\sqrt{((z+a)^2+r^2)})]. \tag{5.4}$$

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REFERENCES

1) Boumans, Colloquium Spectroscopicum Internationale, May 1956, Amsterdam.