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Correction of the Diffusion Equation

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A test problem is investigated and indicate that the conventional foundation of Fick's law and the resulting diffusion equation admit mass transfer at relatively high velocity. This contradicts nature and two independent corrections are made:

1. The front beyond which matier cannot reach; advances with a characteristic speed dependent on the diffusing substance and the medium;
2. Relativistic type correction in which time dilation and length contraction is taken in consideration.

In both cases solutions are obtained and discussed.

Keywords: diffusion equation, diffusion front, relativistic correction, Stoke's law.

1. Statement of the problem

Consider the one dimensional diffusion field defined by $O \leq x < \infty$ initially free from the diffusing substance i.e. $C(0,x) = 0$ at the instant $t = 0$, a steady concentration $C(t,0) = C_0$ is applied at $x = 0$. Accordingly, the concentration function $C(t,x)$ will be the solution of the one dimensional diffusion equation [1]

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}\,, \tag{1}$$

subject to the prescribed initial and boundary condition. This problem admits solution by similarity [2]

$$C(x,t) = C\left(\eta = \frac{x}{2\sqrt{Dt}}\right)\,;$$

where

$$\frac{\partial}{\partial t} = \frac{d}{d\eta}\frac{\partial\eta}{\partial t} = \frac{x}{2\sqrt{D}}\left(-\frac{1}{2}t^{-\frac{3}{2}}\right)\frac{d}{d\eta} = -\frac{\eta}{2t}\frac{d}{d\eta}\,,$$

$$\frac{\partial}{\partial x} = \frac{d}{d\eta}\frac{\partial \eta}{\partial x} = \frac{1}{2\sqrt{Dt}}\frac{d}{d\eta}\,;$$

Accordingly

$$-\frac{\eta}{2t}\frac{dC}{d\eta} = D\frac{1}{4Dt}\frac{d^2C}{d\eta^2} \quad \text{i.e. } \frac{dp}{p} = -2\eta d\eta\,, \quad p = \frac{dC}{d\eta}\,,$$

then

$$p = k\mathrm{e}^{-\eta^2}$$

and

$$dC = k\mathrm{e}^{-\eta^2}d\eta\,,$$

integrating from $\eta = 0$ $(x = 0)$ to η

$$C = C_o + \bar{k}\,\mathrm{erf}(\eta)\,, \quad \bar{k} = \frac{2k}{\sqrt{\pi}}\,, \text{ at } t = 0 \ (\eta = \infty) \ C = 0\,,$$

implies

$$0 = C_0 + \bar{k}\,\mathrm{erf}(\infty) \quad \text{therefore } \bar{k} = -C_0\,,$$

giving

$$C(x,t) = C_0\left[1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right]. \tag{2}$$

Now consider small time ϵ together with a large distance $\frac{1}{\epsilon}$, therefore

$$C\left(\frac{1}{\epsilon}, \epsilon\right) = C_0\left[1 - \ \mathrm{erf}\left(\frac{1}{2\epsilon\sqrt{D\epsilon}}\right)\right] > 0\,,$$

indicating matter moves with average velocity $\frac{1}{\epsilon^2}$ which can be very large and contradicts nature, whence corrections must be made.

2. First correction (front advance)

We assume in this problem that matter cannot reach beyond a front which advances in the direction of diffusion. Suitable assumption about the concentration and its gradient at this front must be made. Accordingly, Fick's law must be written as – the flux density $\dot{q} = -D\frac{\partial C}{\partial x}u(\chi(t) - x)$ where u the unit step function shown in Figure 1, the diffusion equation (1) will be:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}u\left(\chi(t) - x\right)\,, \quad 0 \le x < \infty\,, \quad t \ge 0\,,$$

$$C(0,t) = C_0\,, \quad C(x,0) = 0\,.$$

To solve this problem we take the Laplace transform on time and the Fourier sine transform on x [3]. The transformed function $\hat{C}$ will satisfy

$$\hat{C} = \frac{D\omega}{s(s + D\omega^2)} + \frac{\hat{F}(s,\omega)}{s + D\omega^2}\,,$$

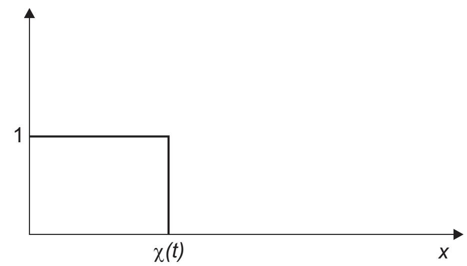

Figure 1

where

$$\hat{F}(s,\omega) = D\left[\left.\frac{\partial C}{\partial x}\right|_{\chi(t)} \sin\left(\omega\chi(t)\right) - \omega C|_{\chi(t)}\cos\left(\omega\chi(t)\right)\right].$$

Inverting transforms gives

$$\frac{C(x,t)}{C_0} = 1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right) + \frac{2}{\pi}\int_0^\infty L^{-1}\frac{\hat{F}(\omega,s)}{s+\omega^2 D}\sin(\omega x)d\omega = \text{part1} + \text{part2}.$$

Part 2 admits convolution integral as:

$$\frac{2}{\pi}D\int_0^\infty\int_0^t \mathrm{e}^{-D\omega^2(t-\tau)}\begin{bmatrix} \left.\frac{\partial C}{\partial x}\right|_{\chi(\tau)}\sin(\omega\chi(\tau)) \\ -\omega C\big|_{\chi(\tau)}\cos(\omega\chi(\tau)) \end{bmatrix} \tag{3}$$

at this stage two possibilities are investigated simultaneously

1) $\left.\frac{\partial C}{\partial x}\right|_{\chi(t)} = 0\,,$

2) $\chi(t) = \nu(t)\,,$ v being a physical constant.

Equation (3) reduces to

$$-\frac{2}{\pi}D\int_0^\infty \omega\sin\omega x\mathrm{e}^{-D\omega^2 t}\int_0^t \mathrm{e}^{D\omega^2\tau}\; C|_{\nu\tau}\cos(\omega\nu\tau)d\tau d\omega\,.$$

The inner integral can be evaluated by parts as

$$C|_{\nu t}\int_0^t \mathrm{e}^{D\omega^2\tau}\cos\omega\nu\tau - \int_0^t\left[\int_0^t \mathrm{e}^{D\omega^2\tau}\cos\omega\nu\tau d\tau\right]\left.\frac{dC}{d\tau}\right|_{\nu t} dt\,,$$

it is easily to show that

$$\left.\frac{dC}{d\tau}\right|_{\nu\tau} = \nu\left.\frac{dC}{dx}\right|_{\nu t} = 0\,,$$

and the inner integral reduces to

$$C|_{\nu t}\,\frac{\mathrm{e}^{D\omega^2 t}\left[D\omega^2\cos\omega\nu t + \omega\nu\sin\omega\nu t\right] - D\omega^2}{\omega^2\left(D^2\omega^2+\nu^2\right)}$$

Accordingly, part 2 reduces to

$$\frac{2}{\pi}\, C|_{\nu t}\left[\frac{\pi}{2}\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu}{D}x+\int_0^\infty\frac{\mathrm{e}^{-D\omega^2 t}\omega\sin\omega x d\omega}{\omega^2+\left(\frac{\nu}{D}\right)^2}\right]$$

giving

$$\frac{C(x,t)}{C_0}=1-\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)+\frac{C|_{\nu t}}{C_0}\left[\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu}{D}x+\frac{2}{\pi}\int_0^\infty\frac{\mathrm{e}^{-D\omega^2 t}\omega\sin\omega x d\omega}{\omega^2+\left(\frac{\nu}{D}\right)^2}\right]$$

This relation gives for $(x=\nu t)$, t

$$\frac{C|_{\nu t}}{C_0}=\frac{1-\mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right)}{1-\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu^2}{D}t-\frac{2}{\pi}\int_0^\infty\frac{\mathrm{e}^{-D\omega^2 t}\omega\sin\omega x d\omega}{\omega^2+\left(\frac{\nu}{D}\right)^2}} \tag{4}$$

therefore

$$\begin{aligned}\frac{C(x,t)}{C_0} &= 1-\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)+\left(1-\mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right)\right)\times\\ &\qquad\left[\frac{\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu}{D}x+\frac{2}{\pi}\int_0^\infty\frac{\mathrm{e}^{-D\omega^2 t}\omega\sin\omega x d\omega}{\omega^2+\left(\frac{\nu}{D}\right)^2}}{1-\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu^2}{D}t-\frac{2}{\pi}\int_0^\infty\frac{\mathrm{e}^{-D\omega^2 t}\omega\sin\omega x d\omega}{\omega^2+\left(\frac{\nu}{D}\right)^2}}\right].\end{aligned} \tag{5}$$

Solutions (4), (5) can be investigated carefully after evaluating the integral involved, however we point out that solution (4) shows

- At $t=0$ the front is at $x=0$ will

$$\frac{C_0}{C_0}=1=\frac{1}{1-0+0}\quad\text{(correct;)}$$

- at $t\to\infty$ the front $\to\infty$

$$0=\frac{0}{1-\infty-0}\quad\text{(correct.)}$$

The integral

$$I=\int_0^\infty\frac{\mathrm{e}^{-Dt\omega^2}\omega\sin\omega x}{\omega^2+\beta^2}d\omega=\frac{1}{2}\int_0^\infty\frac{\mathrm{e}^{-Dt\Omega}\sin\sqrt{\Omega}x}{\Omega+\beta^2}d\Omega\,.$$

Then

$$\frac{dI}{d(Dt)}=\frac{1}{2}\int_0^\infty\frac{-\Omega\mathrm{e}^{-Dt\Omega}\sin\sqrt{\Omega}x}{\Omega+\beta^2}d\Omega=\beta^2 I-\frac{1}{2}\int_0^\infty\mathrm{e}^{-Dt\Omega}\sin\sqrt{\Omega}x d\Omega\,.$$

Let

$$J=\int_0^\infty\mathrm{e}^{-Dt\Omega}\sin\sqrt{\Omega}x d\Omega\,,$$

gives

$$\frac{\partial J}{\partial t} = D\frac{\partial^2 J}{\partial x^2}\,, \quad J(\infty, x) = J(t, 0) = 0\,.$$

The solution is

$$J = \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$$

and

$$I = \frac{1}{2}\mathrm{e}^{\frac{\nu^2}{D}t}\int_0^\infty \mathrm{e}^{-\frac{\nu^2}{D}t}\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)dt$$

by parts, we obtain

$$I = \frac{D}{2\nu^2}\left[\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) - \frac{1}{\sqrt{\pi}}\mathrm{e}^{\frac{\nu^2}{D}t}\frac{x}{2\sqrt{D}}\int_t^\infty t^{-\frac{3}{2}}\mathrm{e}^{-\left(\frac{\nu^2}{D}t+\frac{x^2}{4Dt}\right)}dt\right]\,.$$

Since $\frac{\nu^2}{D}t = \frac{x^2}{4Dt}$ at $t = \frac{x}{2\nu}$ the integral

$$\int_t^\infty t^{-\frac{3}{2}}\mathrm{e}^{-\left(\frac{\nu^2}{D}t+\frac{x^2}{4Dt}\right)}dt$$

is approximated by

$$\int_t^{\frac{x}{2\nu}} t^{-\frac{3}{2}}\mathrm{e}^{-\frac{x^2}{4Dt}}dt + \int_{\frac{x}{2\nu}}^\infty t^{-\frac{3}{2}}\mathrm{e}^{-\frac{\nu^2}{D}t}dt\,.$$

For

$$I_1 = \int_t^{\frac{x}{2\nu}} t^{-\frac{3}{2}}\mathrm{e}^{-\frac{x^2}{4Dt}}dt = -\frac{2\sqrt{D}}{x}\int_{\frac{x^2}{4Dt}}^{\frac{x\nu}{2D}} \tau^{-\frac{1}{2}}\mathrm{e}^{-\tau}d\tau \approx \frac{2\sqrt{D}}{x}\ln\left(\frac{x}{2\sqrt{t}}\right)\,.$$

For

$$I_2 = \int_{\frac{x}{2\nu}}^\infty t^{-\frac{3}{2}}\mathrm{e}^{-\frac{\nu^2}{D}t}dt = \frac{\nu}{\sqrt{D}}\int_{\frac{x\nu}{2D}}^\infty \tau^{-\frac{3}{2}}\mathrm{e}^{-\tau}d\tau \approx \frac{2\sqrt{D}}{x}\,.$$

Then we can write

$$I \approx \frac{D}{2\nu^2}\left[\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right) - \mathrm{e}^{\frac{\nu^2}{D}t}\left(1 + \ln\frac{x}{2\nu t}\right)\right]\,.$$

Let

$$\Gamma = \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\mathrm{e}^{-\frac{\nu^2}{D}t} - \ln\frac{x}{2\nu t}\,.$$

The integral

$$I = \begin{cases} = 0 & \text{if} \quad \Gamma = 1 \\ > 0 & \text{if} \quad \Gamma > 1 \\ < 0 & \text{if} \quad \Gamma < 1\,. \end{cases}$$

Substituting in (4)

$$\frac{C|_{\nu t}}{C_0} = \frac{1 - \mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right)}{1 - \mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu^2}{D}t - \frac{2}{\pi}\frac{D}{2\nu^2}\left[\mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right) - \mathrm{e}^{\frac{\nu^2}{D}t}\left(1 + \ln\frac{1}{2}\right)\right]} \tag{6}$$

Substituting in (5)

$$\begin{aligned}\frac{C(x,t)}{C_0} &= 1-\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)+\left(1-\mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right)\right)\times \\ &\left[\frac{\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu^2}{D}x+\frac{2}{\pi}\frac{D}{2\nu^2}\left[\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)-\mathrm{e}^{\frac{\nu^2}{D}t}\left(1+\ln\frac{x}{2\nu t}\right)\right]}{1-\mathrm{e}^{\frac{\nu^2}{D}t}\sinh\frac{\nu^2}{D}t-\frac{2}{\pi}\frac{D}{2\nu^2}\left[\mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right)-\mathrm{e}^{\frac{\nu^2}{D}t}\left(1+\ln\frac{1}{2}\right)\right]}\right]\end{aligned} \tag{7}$$

The bracket

$$\mathrm{erf}\left(\frac{\nu t}{2\sqrt{Dt}}\right)-\mathrm{e}^{\frac{\nu^2}{D}t}\left(1+\ln\frac{1}{2}\right)\;;\quad \alpha^2=\frac{\nu^2 t}{D}=\mathrm{erf}(\alpha)-\mathrm{e}^{2\alpha^2}\left(1+\ln\frac{1}{2}\right).$$

The bracket is positive if $\mathrm{e}^{-2\alpha^2}\,\mathrm{erf}(\alpha) > 1+\ln\frac{1}{2}$ and is negative if $\mathrm{e}^{-2\alpha^2}\,\mathrm{erf}(\alpha) < 1+\ln\frac{1}{2}$ and if $\mathrm{e}^{-2\alpha^2}\,\mathrm{erf}(\alpha) = 0.307$ gives $\alpha_0 = \frac{\nu^2 t_0}{D} = 0.38227$. Consequently, it is essential that the denominator is negative and $\frac{C(x,t)}{C_0}$ will be $< 1-\mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)$ and it is not necessary for x to reach ∞ that $C\to 0$.

3. Second correction

Relativistic proper time and space if the frame x,t of the equation

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}\,,$$

are the proper time and position, then in the stationary frame the equation should read

$$\frac{\partial C}{\partial t}=D\frac{\partial^2 C}{\partial x^2}\left(1-\frac{\nu^2}{c^2}\right)^{\frac{3}{2}}\,,$$

Lorentz transformation [4]. If C is observed in the neighborhood of a typical particle (the neighborhood size is determined by the mean free path) then x,t are related by

$$\frac{d}{dt}=\nu\frac{d}{dx}\,,$$

where ν, is the velocity of the particle and in this neighborhood

$$\nu\frac{dC}{dx}=D\frac{d^2C}{dx^2}\left(1-\frac{\nu^2}{c^2}\right)^{\frac{3}{2}}\,, \tag{8}$$

the moving particle has the equation of motion (free diffusion)

$$m\nu\frac{d\nu}{dx}=-6\pi\mu a\nu\,,\ \text{Stoke's law [5].}$$

Here, m is mass of particle, a – diameter of particle (considered spherical), μ is viscosity of medium which gives

$$\nu=\nu_0-\frac{6\pi\nu a}{m}(x-x_0)\,. \tag{9}$$

Let $p = \frac{dC}{dx}$, equation (1) can be written in the form

$$\frac{dp}{p} = -\frac{m}{6\pi\mu aD}\frac{\nu d\nu}{\left(1-\frac{\nu^2}{c^2}\right)^{\frac{3}{2}}} \,,$$

integrate

$$\ln\frac{p}{p_0} = -2\frac{mc^2}{6\pi\mu aD}\left[\frac{1}{\sqrt{1-\frac{\nu^2}{c^2}}} - \frac{1}{\sqrt{1-\frac{\nu_0^2}{c^2}}}\right] ,$$

then

$$p \approx p_0\left[1 - 2\frac{mc^2}{6\pi\mu aD}\left[\frac{1}{\sqrt{1-\frac{\nu^2}{c^2}}} - \frac{1}{\sqrt{1-\frac{\nu_0^2}{c^2}}}\right]\right] ,$$

retaining only the first binomial expansion. But

$$\frac{dC}{dx} = -\frac{dC}{d\nu}\frac{6\pi\mu a}{m} \,,$$

therefore

$$C(\nu) - C(\nu_0) = p_0\left[-(\nu-\nu_0)\frac{mc}{6\pi\mu a} + 2\frac{mc^2}{(6\pi\mu a)^2 D}\left(\frac{\nu-\nu_0}{\sqrt{1-\frac{\nu_0^2}{c^2}}} - (\nu-\nu_0)\right)\right]$$

and

$$C(x) = C(x_0) - |p_0|\left\{(x-x_0)\left[1 + 2\frac{mc^2}{6\pi\mu aD}\left(\frac{1}{\sqrt{1-\frac{\nu_0^2}{c^2}}} - 1\right)\right]\right\}$$

Test problem $x_0 = 0$, $C(x_0) = 1$

$$C(x) = 1 - |p_0|(x)\left\{\left[1 + 2\frac{mc^2}{6\pi\mu aD}\left(\frac{1}{\sqrt{1-\frac{\nu_0^2}{c^2}}} - 1\right)\right]\right\} . \tag{10}$$

Two physical constraints on C exist namely; $C \geq 0$, $C \leq 1$, indicating x_{max} for $C = 0$ such that

$$x_{max} = \frac{1}{|p_0|\left\{\left[1 + \frac{2mc^2}{6\pi\mu aD}\left(\frac{1}{\sqrt{1-\frac{\nu_0^2}{c^2}}} - 1\right)\right]\right\}} . \tag{11}$$

It is clear that if $\frac{\nu_0}{c}$ correction is neglected $x \to \infty$, otherwise we have a finite x_{max}.

4. Example

Fine carbon particles from rocket exhaust in ambient air [6]. $a = 10^{-6}$ m, $m = 12\times1.67\times10^{-27}$ kg, $D = 0.52\times10^{-5}$ m^2/s, $\mu = 2.57\times10^{-5}$ kg s/m^2, $c = 3\times10^8$ m/s, $\nu_0 = 10^4$ m/s (escape velocity).

$$x_{max} = \frac{1}{|p_0|\left\{\left[1+\frac{2mc^2}{6\pi\mu aD}\left(\frac{1}{\sqrt{1-\frac{\nu_0^2}{c^2}}}-1\right)\right]\right\}} = \frac{1}{|p_0|\times 1.25\times 10^2}\,.$$

The dust will spread a distance 1000 m, if $|p_0| = 0.08$.

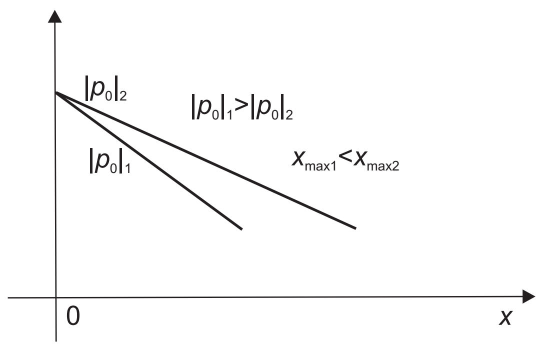

Figure 2

Fig. 2 shows that if $|p_0|$ increases then x_{max} decreases.

5. Conclusions

In the two suggested corrections we succeeded in finding x_{max} where it is not necessary for x to reach ∞ that C should tend to zero. It might be argued that the relativistic correction may not be acceptable since actual velocities in diffusion are far below speed of light. However we point out that from the qualitative point of view the relativistic correction proved possible. The front corrections adds to the problem of diffusion another physical constant i.e. the front speed ν which will depend on both the medium and the diffusing substance and must be determined together with the diffusion constant D.

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