The Diffusion Equation

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1 Swarms

Fundamentals

1° We imagine a Swarm of N particles in $\mathbf{R}^3$, in random motion. We describe the distribution of the particles in the Swarm by the number density function ν:

$$\nu(t,\mathbf{r}) \equiv \nu(t,x,y,z)$$

where the nonnegative number t records time and the vector $\mathbf{r} = (x,y,z)$ locates position. We measure time in seconds (sec) and length in micrometers (μm). For any time t and for any region B in $\mathbf{R}^3$:

$$\iiint_B \nu(t,\mathbf{r})d\mathbf{r} \equiv \iiint_B \nu(t,x,z)dxdydz$$

is the number at time t of the particles in the Swarm having position $\mathbf{r}$ in B. Consequently, ν carries the units $(\mu m)^{-3}$. Of course:

$$\iiint_{\mathbf{R}^3} \nu(t,\mathbf{r})d\mathbf{r} = N$$

We describe the flow of the particles in the Swarm by the velocity density function $\mathbf{j}$:

$$\mathbf{j}(t,\mathbf{r}) \equiv (f(t,x,y,z), g(t,x,y,z), h(t,x,y,z))$$

For any time t and for any region B in $\mathbf{R}^3$:

$$\iiint_B \mathbf{j}(t,\mathbf{r})d\mathbf{r}$$

is the total velocity at time t of the particles in the Swarm having position $\mathbf{r}$ in B. The components of $\mathbf{j}$ carry the units $sec^{-1}(\mu m)^{-2}$.

2° Let B be a ball in $\mathbf{R}^3$ and let S be its surface. Let us introduce the surface integral:

$$\phi(t) \equiv \iint_S \mathbf{j}(t,\mathbf{r}) \bullet \boldsymbol{\sigma}(d\mathbf{r})$$

In the foregoing expression:

$$\boldsymbol{\sigma}(d\mathbf{r}) \equiv \sigma(d\mathbf{r})\mathbf{n}(\mathbf{r})$$

where $\sigma(d\mathbf{r})$ is the area of a small patch of S at $\mathbf{r}$ and $\mathbf{n}(\mathbf{r})$ is the (outward directed) unit vector normal to S at $\mathbf{r}$. The dot product:

$$\mathbf{j}(t,\mathbf{r}) \bullet \mathbf{n}(\mathbf{r})$$

is the component of $\mathbf{j}(t,\mathbf{r})$ in the direction at $\mathbf{r}$ defined by $\mathbf{n}(\mathbf{r})$. We interpret $\phi(t)$ to be the rate at time t at which the particles leave the ball B. Of course, $\phi(t)$ may be negative.

3° By the Theorem of Gauss, we may transform the surface integral as follows:

$$\iint_S \mathbf{j}(t,\mathbf{r}) \bullet \boldsymbol{\sigma}(d\mathbf{r}) = \iiint_B (\nabla \bullet \mathbf{j})(t,\mathbf{r})d\mathbf{r}$$

where $\nabla \bullet \mathbf{j}$ is the *divergence* of $\mathbf{j}$:

$$(\nabla \bullet \mathbf{j})(t,\mathbf{r}) \equiv \frac{\partial}{\partial x}f(t,x,y,z) + \frac{\partial}{\partial y}g(t,x,y,z) + \frac{\partial}{\partial z}h(t,x,y,z)$$

We infer that:

$$\phi(t) = \iiint_B (\nabla \bullet \mathbf{j})(t,\mathbf{r})d\mathbf{r}$$

4° Naturally, at any time t, the rate of increase of the number of particles in B must equal the negative of the rate at which the particles leave B. That is:

$$\frac{d}{dt}\iiint_B \nu(t,\mathbf{r})d\mathbf{r} = -\phi(t)$$

Hence:

$$\iiint_B \Big[\frac{\partial}{\partial t}\nu(t,\mathbf{r}) + (\nabla \bullet \mathbf{j})(t,\mathbf{r})\Big]d\mathbf{r} = 0$$

Since B may be any ball in $\mathbf{R}^3$, we **conclude** that, for any time t and for any position $\mathbf{r}$ in $\mathbf{R}^3$:

$$(CE) \qquad \frac{\partial}{\partial t}\nu(t,\mathbf{r}) = -(\nabla \bullet \mathbf{j})(t,\mathbf{r})$$

The foregoing relation, called the Continuity Equation, is the first of the three fundamental elements of our study.

Diffusion: the Equation

5° The Continuity Equation is a relation of consistency between the density functions ν and $\mathbf{j}$. It reflects no special assumption about the motion of the Swarm. At this point, however, we introduce a special assumption with far reaching effects:

(∘) the Swarm seeks, by its motion, to establish uniform distribution of its particles as rapidly as possible

Under this assumption, one says that the Swarm undergoes *diffusion*.

6° To express the assumption precisely, we require the *gradient* $\nabla\nu$ of ν:

$$(\nabla\nu)(t,\mathbf{r}) \equiv \big(\frac{\partial}{\partial x}\nu(t,x,y,z), \frac{\partial}{\partial y}\nu(t,x,y,z), \frac{\partial}{\partial z}\nu(t,x,y,z)\big)$$

By elementary argument, one may show that the vector $(\nabla\nu)(t,\mathbf{r})$ defines, at time t, the direction at $\mathbf{r}$ of greatest increase in ν.

7° Let δ be a positive number. Let us **assume** that, for any time t and for any position $\mathbf{r}$ in $\mathbf{R}^3$:

$$(FE) \qquad \mathbf{j}(t,\mathbf{r}) = -\delta(\nabla\nu)(t,\mathbf{r})$$

The foregoing relation, called Fick's Equation, is the second of the three fundamental elements of our study. It expresses, in simplest form, the special assumption (∘) about the motion of the Swarm.

8° The number δ is called the *diffusion coefficient*. It carries the units of $(\mu m)^2 sec^{-1}$. It serves both as a conversion factor and as a measure of the rate at which the Swarm approaches uniform distribution.

9° In context of experiment, the Diffusion Coefficient δ is a characteristic of the medium in which the Swarm moves.

10° Combining (CE) and (FE), we find that:

$$\frac{\partial}{\partial t}\nu(t,\mathbf{r}) = \delta(\nabla \bullet \nabla\nu)(t,\mathbf{r}) \equiv \delta(\nabla^2\nu)(t,\mathbf{r})$$

where $\nabla^2\nu$ is the *laplacian* of ν:

$$(\nabla^2\nu)(t,\mathbf{r}) \equiv \frac{\partial^2}{\partial x^2}\nu(t,x,y,z) + \frac{\partial^2}{\partial y^2}\nu(t,x,y,z) + \frac{\partial^2}{\partial z^2}\nu(t,x,y,z)$$

Now we may **infer** that, for any time t and for any position $\mathbf{r}$ in $\mathbf{R}^3$:

$$(DE) \qquad \frac{\partial}{\partial t}\nu(t,\mathbf{r}) = \delta(\nabla^2\nu)(t,\mathbf{r})$$

The foregoing relation, called the Diffusion Equation, is the last of the three fundamental elements of our study.

2 Simple Diffusion

11° Let us turn to the problem of solving the Diffusion Equation and to the problem of measuring the Diffusion Coefficient.

Fourier Transforms

12° We require the dual relations between functions and their Fourier Transforms:

$$\hat{\alpha}(\mathbf{q}) = \frac{1}{(2\pi)^{3/2}}\iiint_{\mathbf{R}^3} exp(-i\mathbf{q}\bullet\mathbf{r})\alpha(\mathbf{r})d\mathbf{r}$$
$$\alpha(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\iiint_{\mathbf{R}^3} exp(+i\mathbf{q}\bullet\mathbf{r})\hat{\alpha}(\mathbf{q})d\mathbf{q}$$

In this context, α and $\hat{\alpha}$ are complex valued functions of the position vector $\mathbf{r} \equiv (x,y,z)$ and of the *dual* position vector $\mathbf{q} \equiv (u,v,w)$, respectively. The components of $\mathbf{q}$ carry the units $(\mu m)^{-1}$. One refers to $\hat{\alpha}$ as the Fourier Transform of α and to α itself as the Inverse Fourier Transform of $\hat{\alpha}$.

13° In turn, we require a remarkable example: the function β which coincides with its own Fourier Transform:

$$\beta(\mathbf{r}) = exp(-\frac{1}{2}\mathbf{r}\bullet\mathbf{r})$$
$$\hat{\beta}(\mathbf{q}) = exp(-\frac{1}{2}\mathbf{q}\bullet\mathbf{q})$$

It is no accident that β is (essentially) the density function for the standard Normal Distribution in Probability Theory.

14° Finally, we require a basic relation between Fourier Transforms and Convolutions. Let α_1 and α_2 be complex valued functions of the position vector $\mathbf{r}$. We form a new function $\alpha_1 * \alpha_2$, called the *convolution* of α_1 and α_2, as follows:

$$(\alpha_1 * \alpha_2)(\mathbf{r}) \equiv \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} \alpha_1(\mathbf{r}-\mathbf{s})\alpha_2(\mathbf{s})d\mathbf{s}$$

We have introduced the position vector $\mathbf{s} \equiv (a, b, c)$ to represent the variable of integration. By straightforward computation, one may show that:

$$(\alpha_1 * \alpha_2)\hat{}(\mathbf{q}) = \hat{\alpha}_1(\mathbf{q})\hat{\alpha}_2(\mathbf{q})$$

That is, the Fourier Transform of the convolution of α_1 and α_2 is the product of the Fourier Transforms of α_1 and α_2.

Diffusion: the Solution

15° Now let us apply the Fourier Transform to the number density function ν:

$$\begin{aligned} \hat{\nu}(t,\mathbf{q}) &= \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} exp(-i\mathbf{q}\bullet\mathbf{r})\nu(t,\mathbf{r})d\mathbf{r} \\ \nu(t,\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} exp(+i\mathbf{q}\bullet\mathbf{r})\hat{\nu}(t,\mathbf{q})d\mathbf{q} \end{aligned}$$

In the foregoing relations, we regard the time t as a parameter. By interchanging derivative and integral, we find that:

$$\begin{aligned} \frac{\partial}{\partial t}\nu(t,\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} exp(+i\mathbf{q}\bullet\mathbf{r})\frac{\partial}{\partial t}\hat{\nu}(t,\mathbf{q})d\mathbf{q} \\ (\nabla^2\nu)(t,\mathbf{r}) &= \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} exp(+i\mathbf{q}\bullet\mathbf{r})(-\mathbf{q}\bullet\mathbf{q})\hat{\nu}(t,\mathbf{q})d\mathbf{q} \end{aligned}$$

Hence:

$$\begin{aligned} \frac{\partial}{\partial t}\hat{\nu}(t,\mathbf{q}) &= \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} exp(-i\mathbf{q}\bullet\mathbf{r})\frac{\partial}{\partial t}\nu(t,\mathbf{r})d\mathbf{r} \\ -(\mathbf{q}\bullet\mathbf{q})\hat{\nu}(t,\mathbf{q}) &= \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} exp(-i\mathbf{q}\bullet\mathbf{r})(\nabla^2\nu)(t,\mathbf{r})d\mathbf{r} \end{aligned}$$

Consequently:

$$\frac{\partial}{\partial t}\nu(t,\mathbf{q}) = \delta(\nabla^2\nu)(t,\mathbf{r}) \quad \text{iff} \quad \frac{\partial}{\partial t}\hat{\nu}(t,\mathbf{q}) = -\delta(\mathbf{q}\bullet\mathbf{q})\hat{\nu}(t,\mathbf{q})$$

16° By the foregoing computations, we have passed the Diffusion Equation through the "Fourier Mirror," transforming a partial differential equation of relatively complicated form into an ordinary differential equation of altogether simple form. Indeed, by inspection, we see that:

$$\hat{\nu}(t, \mathbf{q}) = exp(-\delta(\mathbf{q} \bullet \mathbf{q})t))\hat{\nu}(0, \mathbf{q})$$

Referring to article 13°, we change scale in β:

$$\gamma(t, \mathbf{r}) \equiv \frac{1}{(2\delta t)^{3/2}} exp(-\frac{1}{2}\frac{1}{2\delta t}\mathbf{r} \bullet \mathbf{r})$$

with the following good effect:

$$\hat{\gamma}(t, \mathbf{q}) = exp(-\delta(\mathbf{q} \bullet \mathbf{q})t)$$

Referring to article 14°, we conclude that:

$$(\bullet) \qquad \nu(t, \mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} \gamma(t, \mathbf{r} - \mathbf{s})\nu(0, \mathbf{s})d\mathbf{s}$$

The foregoing relation describes the development of the number density function for the Swarm, from its state at time 0 to its state at time t.

17° For precision of expression, let us introduce the following notational conventions:

$$\nu_t(\mathbf{r}) \equiv \nu(t, \mathbf{r})$$
$$\gamma_t(\mathbf{r}) \equiv \gamma(t, \mathbf{r})$$

Now our solution of the Diffusion Equation takes the form:

$$(\bullet) \qquad \nu_t = \gamma_t * \nu_0$$

18° One should note that:

$$\kappa(t, \mathbf{r}) \equiv \frac{1}{(2\pi 2\delta t)^{3/2}} exp(-\frac{1}{2}\frac{1}{2\delta t} r \bullet \mathbf{r}) = \frac{1}{(2\pi)^{3/2}}\gamma(t, \mathbf{r})$$

is the density function for the Normal Distribution on $\mathbf{R}^3$, having mean $\mathbf{0}$ and variance $2\delta t$. Obviously:

$$\nu(t, \mathbf{r}) = \iiint_{\mathbf{R}^3} \kappa(t, \mathbf{r} - \mathbf{s})\nu(0, \mathbf{s})d\mathbf{s}$$

Mean Square Displacement

19° For applications, we require a good estimate of the Diffusion Constant δ. To that end, we introduce the *mean square displacement*:

$$m(t) \equiv \frac{1}{N} \iiint_{\mathbf{R}^3} (\mathbf{r} \bullet \mathbf{r})\, \nu(t, \mathbf{r}) d\mathbf{r}$$

where, as usual, t is the time. We contend that:

$$(*) \qquad m(t) = m(0) + 6\delta t$$

By the foregoing relation, one may proceed to make estimates of δ in the laboratory.

20° To prove the contention, we return to article 15°. Interchanging ν and $\hat{\nu}$, we obtain:

$$(\nabla^2 \hat{\nu})(t, \mathbf{0}) = -\frac{1}{(2\pi)^{3/2}} \iiint_{\mathbf{R}^3} (\mathbf{r} \bullet \mathbf{r})\, \nu(t, \mathbf{r}) d\mathbf{r}$$

Hence:

$$m(t) = -\frac{(2\pi)^{3/2}}{N} (\nabla^2 \hat{\nu})(t, \mathbf{0})$$

Of course, we know that:

$$\hat{\nu}(t, \mathbf{q}) = \hat{\gamma}(t, \mathbf{q}) \hat{\nu}(0, \mathbf{q}) \quad \text{and} \quad \hat{\gamma}(t, \mathbf{q}) = exp(-\delta(\mathbf{q} \bullet \mathbf{q})t)$$

Hence:

$$\begin{aligned} &(\nabla^2 \hat{\nu})(t, \mathbf{q}) \\ &\quad = (\nabla^2 \hat{\gamma})(t, \mathbf{q}) \hat{\nu}(0, \mathbf{q}) + (\nabla \hat{\gamma})(t, \mathbf{q}) \bullet (\nabla \hat{\nu})(0, \mathbf{q}) + \hat{\gamma}(t, \mathbf{q})(\nabla^2 \hat{\nu})(0, \mathbf{q}) \end{aligned}$$

and:

$$\begin{aligned} (\nabla \hat{\gamma})(t, \mathbf{q}) &= -2\delta t\, exp(-\delta(\mathbf{q} \bullet \mathbf{q})t)\, \mathbf{q} \\ (\nabla^2 \hat{\gamma})(t, \mathbf{q}) &= \quad 4\delta^2 t^2 (\mathbf{q} \bullet \mathbf{q}) exp(-\delta(\mathbf{q} \bullet \mathbf{q})t) - 6\delta t\, exp(-\delta(\mathbf{q} \bullet \mathbf{q})t) \end{aligned}$$

Therefore:

$$\begin{aligned} m(t) &= -\frac{(2\pi)^{3/2}}{N} (\nabla^2 \hat{\nu})(t, \mathbf{0}) \\ &= -(\nabla^2 \hat{\gamma})(t, \mathbf{0}) \frac{(2\pi)^{3/2}}{N} \hat{\nu}(0, \mathbf{0}) - \frac{(2\pi)^{3/2}}{N} (\nabla^2 \hat{\nu})(0, \mathbf{0}) \\ &= \quad 6\delta t + m(0) \end{aligned}$$

3 Prospects

Particle Motion

21° One should study the following time-dependent Ordinary Differential Equation, defined by the velocity density function $\mathbf{j}$:

$$\frac{\partial}{\partial t}\bar{\mathbf{r}}(t, \mathbf{r}) = \mathbf{j}(t, \bar{\mathbf{r}}(t, \mathbf{r}), \qquad \bar{\mathbf{r}}(0, \mathbf{r}) = \mathbf{r}$$

Boundaries

22° In the foregoing study of *simple diffusion*, we have allowed the Swarm to evolve without constraints on its territory. No matter the initial distribution of the particles, the Swarm dissipates toward ever smaller densities over ever larger domains. One should refine the study by incorporating constraints. For instance, one might confine the Swarm to a rectangular box with reflecting or absorbing boundaries.

General Diffusion

23° One should replace the Diffusion Constant δ by a function of time t and position $\mathbf{r}$:

$$\delta(t, \mathbf{r})$$

The relation between the support of δ and a putative constraint on territory would be interesting.