Note: Aris-Taylor dispersion from single-particle point of view

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When a point Brownian particle diffuses in a straight circular tube of radius R in the presence of a laminar stationary flow of the liquid (Poiseuille flow), particle's effective diffusion coefficient along the tube axis, D_{eff}, is given by

$$D_{eff} = D + \frac{\bar{v}^2 R^2}{48D}, \tag{1}$$

where D is the particle diffusion coefficient in the absence of flow, and $\bar{v}$ is the average fluid velocity. The increase of the axial diffusion coefficient, $D_{eff} > D$, is due to the radial diffusion that transports the particle among layers with different axial velocities. Taylor discovered this effect in 1953.[1] Later Aris improved the Taylor theory.[2] In this short note we give a new derivation of the expression for D_{eff} in Eq. (1), which is based on consideration of the axial displacement of a single particle that moves in the plane normal to the tube axis along a given trajectory $\{\mathbf{r}\}_t$. We derive the expression in Eq. (1) by averaging this displacement and its square over different realizations of the trajectory and analyzing the long-time asymptotic behavior of these two moments. To the best of our knowledge our derivation of D_{eff} is quite different from traditional derivations that one can find in the textbooks and original papers.

Consider a laminar steady flow in a straight circular tube of radius R. We use cylindrical polar coordinates (r, θ, z) with the z-axis directed towards the flow. The fluid velocity $v(r)$ monotonically decreases from its maximum value at the center of the tube to zero at $r = R$,

$$v(r) = 2\bar{v}\left(1 - \frac{r^2}{R^2}\right), \quad 0 \le r \le R, \tag{2}$$

where $\bar{v}$ is the average velocity given by

$$\bar{v} = 2\pi \int_0^R v(r) p_{eq}(r) r dr = \frac{2}{R^2}\int_0^R v(r) r dr, \tag{3}$$

and $p_{eq}(r) = 1/(\pi R^2)$.

We use $\{\mathbf{r}\}_t$ as the notation for a two-dimensional particle trajectory in the plane perpendicular to the tube axis observed for time t, $\{\mathbf{r}\}_t = \{\mathbf{r}(t'), 0 \le t' \le t\}$. The particle velocity in the axial direction at time t is

$$\dot{z}(t|\mathbf{r}(t)) = v(r(t)) + f(t), \tag{4}$$

where $f(t)$ is the Gaussian δ-correlated random force with zero mean, $\langle f(t)\rangle = 0$, which satisfies the fluctuation-dissipation theorem, $\langle f(t) f(t')\rangle = 2D\delta(t - t')$. On average this force does not lead to an axial displacement, but leads to the additive contribution $2Dt$ to the mean squared displacement. Force $f(t)$ is responsible for the particle diffusion along the tube axis in the absence of flow, which is represented by the first term in the right-hand side of Eq. (1). The second, non-trivial term in the right-hand side of Eq. (1) is due to the particle motion along the tube radius. With this in mind, hereafter we ignore force $f(t)$. Then displacement of the particle in the axial direction is given by

$$z(t|\{\mathbf{r}\}_t) = \int_0^t v(r(t')|\{\mathbf{r}\}_t) dt'. \tag{5}$$

In what follows we use this displacement to derive the second term in the right-hand side of Eq. (1) by analyzing the long-time asymptotic behavior of the first two moments of the displacement averaged over different realizations of the trajectory $\{\mathbf{r}\}_t$.

Using the identity

$$\int \delta(\mathbf{r} - \mathbf{r}(t)) d\mathbf{r} = 1, \tag{6}$$

we can write Eq. (5) as

$$z(t|\{\mathbf{r}\}_t) = \int v(\mathbf{r}) \left(\int_0^t \delta(\mathbf{r} - \mathbf{r}(t')) dt' \right) d\mathbf{r}. \tag{7}$$

This presentation of the displacement has a transparent physical interpretation. Indeed, $(\int_0^t \delta(\mathbf{r} - \mathbf{r}(t'))dt')d\mathbf{r}$ is the cumulative time spent by the trajectory in the small vicinity of point $\mathbf{r}$, where the particle velocity is $v(\mathbf{r})$. Thus, Eq. (7) gives the displacement as a weighted sum of the cumulative times spent by the trajectory at different points of the tube cross section, using the local velocity, $v(\mathbf{r})$, as a weight factor. Such representation of the displacement is the key step in our approach to the problem.

Averaging Eq. (7) over all trajectories that start from the same point, $\mathbf{r}(0) = \mathbf{r}_0$, we obtain

$$\langle z(t)\rangle_{\mathbf{r}_0} = \langle z(t|\{\mathbf{r}\}_t)\rangle_{\mathbf{r}_0} = \int v(\mathbf{r}) \left(\int_0^t \langle \delta(\mathbf{r} - \mathbf{r}(t'))\rangle_{\mathbf{r}_0} dt' \right) d\mathbf{r}. \tag{8}$$

The averaged δ-function in Eq. (8) is the particle propagator (the Green's function) (Ref. 3) in the plane perpendicular to the tube axis,

$$\langle \delta(\mathbf{r} - \mathbf{r}(t))\rangle_{\mathbf{r}_0} = g(\mathbf{r}, t|\mathbf{r}_0). \tag{9}$$

Therefore, the averaged displacement is

$$\langle z(t)\rangle_{\mathbf{r}_0} = \int v(\mathbf{r})\left(\int_0^t g(\mathbf{r}, t'|\mathbf{r}_0)dt'\right)d\mathbf{r}. \tag{10}$$

Here $(\int_0^t g(\mathbf{r}, t'|\mathbf{r}_0)dt')d\mathbf{r}$ is the mean cumulative time spent by the trajectory, $\{\mathbf{r}\}_t$, in the small vicinity of point $\mathbf{r}$.

The propagator $g(\mathbf{r}, t|\mathbf{r}_0)$ tends to $p_{eq}(\mathbf{r}) = 1/(\pi R^2)$ as $t \to \infty$. Denoting the difference between the propagator and $p_{eq}(\mathbf{r})$ by $u(\mathbf{r}, t|\mathbf{r}_0)$, we can write the propagator as

$$g(\mathbf{r}_2, t|\mathbf{r}_1) = p_{eq}(\mathbf{r}_2) + u(\mathbf{r}_2, t|\mathbf{r}_1). \tag{11}$$

Substituting this into Eq. (10) we obtain

$$\langle z(t)\rangle_{\mathbf{r}_0} = \bar{v}t + \int v(\mathbf{r})\left(\int_0^t u(\mathbf{r}, t'|\mathbf{r}_0)dt'\right)d\mathbf{r}. \tag{12}$$

Since $u(\mathbf{r}, t|\mathbf{r}_0)$ vanishes as $t \to \infty$, at asymptotically long times we have

$$\langle z(t)\rangle_{\mathbf{r}_0} = \bar{v}t + l(\mathbf{r}_0), \quad t \to \infty, \tag{13}$$

where $l(\mathbf{r}_0)$ is given by

$$l(\mathbf{r}_0) = \int v(\mathbf{r})\left(\int_0^\infty u(\mathbf{r}, t|\mathbf{r}_0)dt\right)d\mathbf{r}. \tag{14}$$

As might be expected, the long-time behavior of $\langle z(t)\rangle_{\mathbf{r}_0}$ is the sum of the product $\bar{v}t$ and a constant term that depends on $\mathbf{r}_0$.

Averaging the square of the displacement in Eq. (7) over the trajectories that start from $\mathbf{r}_0$ we obtain

$$\begin{aligned}\langle z^2(t)\rangle_{\mathbf{r}_0} &= \langle[z(t|\{\mathbf{r}\}_t)]^2\rangle_{\mathbf{r}_0} \\ &= 2\int\int v(\mathbf{r}_1)v(\mathbf{r}_2)\left(\int_0^t dt_2\int_0^{t_2}\langle\delta(\mathbf{r}_2 - \mathbf{r}(t_2))\right. \\ &\quad \left.\times\,\delta(\mathbf{r}_1 - \mathbf{r}(t_1))\rangle_{\mathbf{r}_0}dt_1\right)d\mathbf{r}_1 d\mathbf{r}_2.\end{aligned} \tag{15}$$

Similar to Eq. (9) the averaged product of the δ-functions in Eq. (15) is the product of the propagators,

$$\begin{aligned}&\langle\delta(\mathbf{r}_2 - \mathbf{r}(t_2))\delta(\mathbf{r}_1 - \mathbf{r}(t_1))\rangle_{\mathbf{r}_0} \\ &= g(\mathbf{r}_2, t_2 - t_1|\mathbf{r}_1)g(\mathbf{r}_1, t_1|\mathbf{r}_0), \quad t_2 > t_1.\end{aligned} \tag{16}$$

This allows us to write $\langle z^2(t)\rangle_{\mathbf{r}_0}$ in terms of the propagator

$$\begin{aligned}\langle z^2(t)\rangle_{\mathbf{r}_0} &= 2\int\int v(\mathbf{r}_1)v(\mathbf{r}_2)\left(\int_0^t dt_2\int_0^{t_2} g(\mathbf{r}_2, t_2 - t_1|\mathbf{r}_1)\right. \\ &\quad \left.\times\, g(\mathbf{r}_1, t_1|\mathbf{r}_0)dt_1\right)d\mathbf{r}_1 d\mathbf{r}_2.\end{aligned} \tag{17}$$

Asymptotic long-time behavior of $\langle z^2(t)\rangle_{\mathbf{r}_0}$ can be found using Eq. (11),

$$\langle z^2(t)\rangle_{\mathbf{r}_0} = \bar{v}^2t^2 + 2t\left[\bar{v}l(\mathbf{r}_0) + \int v(\mathbf{r})l(\mathbf{r})p_{eq}(\mathbf{r})d\mathbf{r}\right], \quad t \to \infty. \tag{18}$$

Thus we have

$$\begin{aligned}\lim_{t\to\infty}\frac{\langle z^2(t)\rangle_{eq} - \langle z(t)\rangle_{eq}^2}{2t} &= \int v(\mathbf{r})l(\mathbf{r})p_{eq}(\mathbf{r})d\mathbf{r} \\ &= \frac{2}{R^2}\int_0^R v(r)l(r)rdr,\end{aligned} \tag{19}$$

where $l(r)$ is function $l(\mathbf{r})$ averaged over θ. We will see that the integral in the right-hand side is just the second term in the expression for D_{eff}, Eq. (1).

To finish the derivation we take advantage of the fact that the propagator $g(\mathbf{r}, t|\mathbf{r}_0)$ considered as a function of $\mathbf{r}_0$ satisfies

$$\frac{\partial g(\mathbf{r}, t|\mathbf{r}_0)}{\partial t} = D\Delta_{\mathbf{r}_0}g(\mathbf{r}, t|\mathbf{r}_0), \tag{20}$$

where $\Delta_{\mathbf{r}_0}$ is the two-dimensional Laplace operator, with reflecting boundary condition on the tube wall. As a consequence, function $u(\mathbf{r}, t|\mathbf{r}_0)$ satisfies the same equation and boundary condition. Integrating both sides of this equation with respect to time from zero to infinity one obtains the equation for $\int_0^\infty u(\mathbf{r}, t|\mathbf{r}_0)dt$. Multiplying both sides of the resulting equation by $v(\mathbf{r})$ and then integrating over the tube cross section one finds that $l(\mathbf{r}_0)$, Eq. (14), satisfies

$$\frac{D}{r_0}\frac{d}{dr_0}\left(r_0\frac{dl(r_0)}{dr_0}\right) = \bar{v} - v(r_0) = \bar{v}\left(2\frac{r_0^2}{R^2} - 1\right) \tag{21}$$

with the boundary condition $dl(r)/dr|_{r=R} = 0$. In addition, $l(r)$ satisfies the requirement

$$\int_0^R l(r)rdr = 0. \tag{22}$$

This can be obtained using Eq. (14) and the fact that $\int_0^R u(\mathbf{r}_2, t|\mathbf{r}_1)d\mathbf{r}_1 = 0$, which follows from Eq. (11). Integrating Eq. (21) one finds

$$l(r) = \frac{\bar{v}}{24DR^2}(3r^4 - 6R^2r^2 + 2R^4). \tag{23}$$

Substituting this into the integral in Eq. (19) and carrying out the integration one recovers the second term in the expression for D_{eff} given in Eq. (1).

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