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Comment on "Local accumulation times for source, diffusion, and degradation models in two and three dimensions" [J. Chem. Phys. 138, 104121 (2013)]

Adam J. Ellery,[1] Matthew J. Simpson,[1,2,a)] and Scott W. McCue[1,2]
[1]School of Mathematical Sciences, Queensland University of Technology, Brisbane, Australia
[2]Tissue Repair and Regeneration Program, Institute of Health and Biomedical Innovation (IHBI), Queensland University of Technology, Brisbane, Australia

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In a recent paper,[1] Gordon, Muratov, and Shvartsman studied a partial differential equation (PDE) model describing radially symmetric diffusion and degradation in two and three dimensions. They paid particular attention to the *local accumulation time* (LAT), also known in the literature as the *mean action time*,[2–7] which is a spatially dependent timescale that can be used to provide an estimate of the time required for the transient solution to effectively reach steady state. They presented exact results for three-dimensional applications and gave approximate results for the two-dimensional analogue. Here we make two generalizations of Gordon, Muratov, and Shvartsman's work: (i) we present an exact expression for the LAT in *any* dimension and (ii) we present an exact expression for the variance of the distribution. The variance provides useful information regarding the spread about the mean that is not captured by the LAT.[5] We conclude by describing further extensions of the model that were not considered by Gordon, Muratov, and Shvartsman.[1] We have found that exact expressions for the LAT can also be derived for these important extensions.

The model treated by Gordon, Muratov, and Shvartsman[1] is

$$\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial r^2} + \frac{n-1}{r}\frac{\partial c}{\partial r}\right) - kc, \quad R < r < \infty, \tag{1}$$

$$c(r,0) = 0, \quad \left.\frac{\partial c}{\partial r}\right|_{r=R} = -\frac{Q}{D}, \quad \lim_{r\to\infty} c(r,t) = 0, \tag{2}$$

where Q is the flux at $r = R$, D is the diffusivity, and k is the degradation rate. Here, n is the physical dimension; setting $n = 1, 2, 3$ corresponds to one-, two-, and three-dimensional problems, respectively.[1] The steady solution of Eq. (1) is

$$\lim_{t\to\infty} c(r,t) = c_s(r) = \frac{Q}{\gamma D}\frac{\mathrm{K}_{n/2-1}(\gamma r)}{\mathrm{K}_{n/2}(\gamma R)}\left(\frac{r}{R}\right)^{1-n/2}, \tag{3}$$

where $\mathrm{K}_\nu(z)$ is the νth order modified Bessel function of the second kind and $\gamma = \sqrt{k/D}$. Gordon, Muratov, and Shvartsman[1] introduce a complementary cumulative distribution function, $\rho(r,t) = (c_s(r) - c(r,t))/c_s(r)$. We note that $0 < \rho(r,t) < 1$, and that $\rho(r,t)$ monotonically decreases with $\rho(r,0) = 1$ and $\rho(r,t) \to 0$ as $t \to \infty$ so that $\rho(r,t)$ measures the progress of the system towards its steady state. The mean of the associated probability density function, $-\partial\rho/\partial t$, is the LAT[2–12] $\tau(r)$:

$$\tau(r) = -\int_0^\infty t\frac{\partial \rho}{\partial t}\,\mathrm{d}t = \int_0^\infty \rho(r,t)\,\mathrm{d}t. \tag{4}$$

By integrating Eq. (1) from zero to infinity with respect to t, and combining this expression with Eq. (4), we obtain a boundary value problem for $\tau(r)$[4–6] which, using the transformed variable $S_1(r) = \tau(r)c_s(r)$, is

$$\frac{\mathrm{d}^2 S_1}{\mathrm{d}r^2} + \frac{n-1}{r}\frac{\mathrm{d}S_1}{\mathrm{d}r} - \frac{k}{D}S_1 = -\frac{c_s(r)}{D}, \tag{5}$$

$$\left.\frac{\mathrm{d}S_1}{\mathrm{d}r}\right|_{r=R} = 0, \quad \lim_{r\to\infty} S_1(r) = 0. \tag{6}$$

Equations (5) and (6) can be solved for $S_1(r)$ for arbitrary n, and this solution can be re-written to give $\tau(r)$,

$$\tau(r) = \frac{1}{k} - \frac{R}{2\gamma D}\frac{\mathrm{K}_{n/2+1}(\gamma R)}{\mathrm{K}_{n/2}(\gamma R)} + \frac{r}{2\gamma D}\frac{\mathrm{K}_{n/2}(\gamma r)}{\mathrm{K}_{n/2-1}(\gamma r)}. \tag{7}$$

For $n = 1$ and $n = 3$, Eq. (7) relaxes to the expressions given by Gordon, Muratov, and Shvartsman.[1,13] Our first main result is to present the exact solution for $n = 2$,

$$\tau(r) = \frac{r\gamma}{2k}\frac{\mathrm{K}_1(\gamma r)}{\mathrm{K}_0(\gamma r)} - \frac{R\gamma}{2k}\frac{\mathrm{K}_0(\gamma R)}{\mathrm{K}_1(\gamma R)}, \tag{8}$$

which is obtained from Eq. (7) using the relationship $\mathrm{K}_2(z) = \mathrm{K}_0(z) + (2/z)\mathrm{K}_1(z)$.[13]

Gordon, Muratov, and Shvartsman's[1] results dealt exclusively with the mean of a distribution whose probability density function is given by $-\partial\rho/\partial t$. In addition to characterizing the mean of this distribution, we can also calculate the variance[5,6] which is given by

$$V(r) = -\int_0^\infty (t - \tau(r))^2\frac{\partial \rho}{\partial t}\,\mathrm{d}t. \tag{9}$$

Following arguments detailed in our previous work,[5,6] the transformed variable $S_2(r) = (V(r) + \tau(r)^2)c_s(r)$ satisfies

$$\frac{\mathrm{d}^2 S_2(r)}{\mathrm{d}r^2} + \frac{n-1}{r}\frac{\mathrm{d}S_2(r)}{\mathrm{d}r} - \frac{k}{D}S_2(r) = -\frac{2}{D}S_1(r), \tag{10}$$

a)E-mail: matthew.simpson@qut.edu.au

$$\left.\frac{dS_2}{dr}\right|_{r=R} = 0, \quad \lim_{r\to\infty} S_2(r) = 0, \tag{11}$$

which has the exact solution

$$S_2(r) = \alpha r^{1-n/2}K_{n/2-1}(\gamma r) + \beta r^{2-n/2}K_{n/2}(\gamma r) + \frac{QR^{n/2-1}r^{3-n/2}}{4\gamma^3 D^3}\frac{K_{n/2+1}(\gamma r)}{K_{n/2}(\gamma R)}, \tag{12}$$

where

$$\alpha = \frac{R^{n/2}Q}{2\gamma^4 D^3}\left(\frac{R\gamma K_{n/2+1}(\gamma R)}{K_{n/2}(\gamma R)} - \frac{n+6}{2}\right)\frac{K_{n/2+1}(\gamma R)}{K_{n/2}(\gamma R)^2} + \left(\frac{2}{\gamma} - \frac{R^2\gamma}{4}\right)\frac{R^{n/2-1}Q}{\gamma^4 D^3}\frac{1}{K_{n/2}(\gamma R)}, \tag{13}$$

$$\beta = \frac{QR^{n/2-1}}{\gamma^4 D^3}\frac{1}{K_{n/2}(\gamma R)} - \frac{QR^{n/2}}{2\gamma^3 D^3}\frac{K_{n/2+1}(\gamma R)}{K_{n/2}(\gamma R)^2}. \tag{14}$$

For $n = 2$ the solution of Eqs. (10) and (11) is

$$S_2(r) = \frac{QR^2}{2\gamma^3 D^3}\frac{K_0(\gamma r)K_0(\gamma R)^2}{K_1(\gamma R)^3} - \frac{Q(R^2 - r^2)}{4\gamma^3 D^3}\frac{K_0(\gamma r)}{K_1(\gamma R)} - \frac{QR}{2\gamma^3 D^3}\frac{rK_1(\gamma r)K_0(\gamma R)}{K_1(\gamma R)^2} + \frac{Q}{2\gamma^4 D^3}\frac{rK_1(\gamma r)}{K_1(\gamma R)}, \tag{15}$$

which allows us to calculate $V(r)$ since we have $V(r) = S_2(r)/c_s(r) - \tau(r)^2$.

Using the LAT alone to characterize the amount of time required for the transient solution of Eq. (1) to approach steady state neglects any consideration of the spread about the mean of the distribution whose probability density function is given by $-\partial\rho/\partial t$. We can provide additional information about this timescale by calculating the variance of the distribution and defining an important time interval $t(r) \in [\tau(r) - \sqrt{V(r)}, \tau(r) + \sqrt{V(r)}]$, which corresponds to the mean of the distribution plus or minus one standard deviation away from the mean.[6] Illustrative results are given in Fig. 1, which shows the LAT, $\tau(r)$, for $n = 2$ using the new exact expression, Eq. (8). This expression avoids the need for any of the approximations introduced by Gordon, Muratov, and Shvartsman.[1] Furthermore, we also show the critical time interval for this problem, $t(r) \in [\tau(r) - \sqrt{V(r)}, \tau(r) + \sqrt{V(r)}]$, which provides an estimate of the time interval required for the transient solution of Eq. (1) to asymptote to the corresponding steady state solution.[6]

We conclude by discussing further possible extensions. Gordon, Muratov, and Shvartsman[1] considered Eq. (1) on $R < r < \infty$, which deals with diffusion and degradation on the outside of a cylinder ($n = 2$) or sphere ($n = 3$). It is also possible to arrive at exact expressions for $\tau(r)$ and $V(r)$ for several related problems where we consider Eq. (1) on a finite domain, $R_1 < r < R_2$. There are many practical applications of such extensions. For example, with $n = 3$ and $R_1 = 0$, this model has been used to study diffusion and degradation of oxygen in a spherical cell.[14] Alternatively, with $n = 2$, $c(r, 0) = c_0$ and $c(R_2, t) = c_0$ for $c_0 > 0$, Eq. (1) on the annulus $R_1 < r < R_2$ models pumping tests that are used to measure field-scale parameters that govern the motion of fluid through an aquifer.[15] We would also like to point out that all results presented and discussed here, in addition to the results considered by Gordon, Muratov, and Shvartsman,[1] can be further generalized to consider an additional constant production or decay term in Eq. (1) where the degradation term, given by $-kc$, is generalized to $-kc + k_0$, where k_0 is some constant. For this additional class of problems it is also possible to calculate expressions for $\tau(r)$ and $V(r)$. We do not present expressions for $\tau(r)$ and $V(r)$ for any of these extensions here to keep this Comment as succinct as possible.

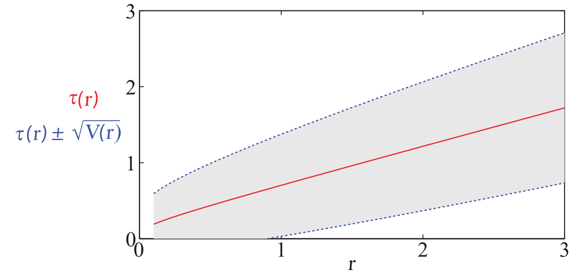

FIG. 1. The red (solid) curve shows the LAT, $\tau(r)$, for $k = D = 1$, $R = 0.1$, and $n = 2$. An important time interval for this transition,[6] $t(r) \in [\tau(r) - \sqrt{V(r)}, \tau(r) + \sqrt{V(r)}]$, is shaded in gray. The upper and lower blue (dotted) curves that enclose the time interval correspond to $\tau(r) \pm \sqrt{V(r)}$, respectively.

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