Asymptotically short term behavior of solutions to one dimensional diffusion processes

by

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Consider the problem of solving the diffusion equation

$$(1)\qquad \left\{ \begin{array}{c} u_t = \frac{\partial}{\partial x}\left(p(x)u_x\right), \;\; 0<x<\pi, \;\; t>0 \\ u(0,t)=u(\pi,t)=0, \;\; t>0 \\ u(x,0)=u_0(x) \end{array} \right\}$$

where $p(x)$ is a smooth, positive function on $[0,\pi]$ and $u_0 \in L^1\left((0,\pi),R\right)$. If we define the operator

$$A : D(A) \to L^1\left((0,\pi),R\right)$$

via

$$A(w) = \frac{d}{dx}\left(p(x)w_x\right)$$

for all

$$w \in D(A) = W^{2,1}\left((0,\pi),R\right) \cap W_0^{1,1}\left((0,\pi),R\right),$$

then A is the infinitesimal generator of an analytic semi-group $\{T(t)\}_{t\geq 0}$ on L^1 (cf. Pazy [10]). Furthermore, the unique solution of (1) is given by

$$u(\cdot,t) = T(t)\left(u_0\right).$$

In addition, if $u_0 \in D\left(A\right)$ then

$$\lim_{t\to 0^+} \frac{T(t)\left(u_0\right) - u_0}{t} = A(u_0).$$

That is,

$$\lim_{t\to 0^+} \frac{u - u_0}{t} = A(u_0),$$

with the limit understood in the L^1 sense. This limit gives information related to the asymptotically short term behavior of the solution to (1) in the case when $u_0 \in D(A)$.

Our primary interest in this work is the short term behavior of the solution to (1) when $u_0 \notin D(A)$. We restrict our attention to the case when u_0 is a smooth function on $[0,\pi]$. For such functions, $u_0 \notin D(A)$ if and only if either $u_0(0) \neq 0$ or $u_0(\pi) \neq 0$. In this case, the short term asymptotic behavior is not immediately transparent. However, we don't have to look far to find useful clues. To this end, we consider a related problem. Let $v_0 \in C^2\left([0,\infty),R\right) \cap L^1\left((0,\infty),R\right)$ and consider the solution to the diffusion equation given by

$$\left\{ \begin{array}{l} v_t = v_{xx}, \;\; 0<x, \;\; t>0 \\ v(0,t)=0, \;\; t>0 \\ v(x,0)=v_0(x) \end{array} \right\}$$

We can write the solution explicitly in the form

$$(2) \qquad v(x,t) = \frac{1}{2\sqrt{\pi t}} \int_0^\infty \left(e^{\left(-(x-y)^2/(4t)\right)} - e^{\left(-(x+y)^2/(4t)\right)} \right) v_0(y)\, dy.$$

This allows us to give an explicit formula for

$$\lim_{t\to 0^+} \frac{\int_0^\infty \left(v_0(x) - v(x,t)\right)\, dx}{\sqrt{t}}.$$

In fact, a simple calculation involving (2), a change of variables and l'Hospital's rule yields

$$\lim_{t\to 0^+} \frac{\int_0^\infty \left(v_0(x) - v(x,t)\right)\, dx}{\sqrt{t}} = \frac{2v_0(0)}{\sqrt{\pi}}.$$

More generally, when $d > 0$, the solution to the system

$$\left\{ \begin{array}{l} v_t = dv_{xx}, \ \ 0 < x, \ \ t > 0 \\ v(0,t) = 0, \ \ t > 0 \\ v(x,0) = v_0(x) \end{array} \right\}$$

satisfies

$$\lim_{t\to 0^+} \frac{\int_0^\infty \left(v_0(x) - v(x,t)\right)\, dx}{\sqrt{t}} = \frac{2\sqrt{d}\, v_0(0)}{\sqrt{\pi}}.$$

The primary result of this work is an extension of this limit formula for solutions to (1).

Our motivation for this work is a mathematical modelling problem associated with waste disposal. The ultimate purpose of proper waste disposal is to discard unwanted materials in a manner which protects the public health and the environment from unwanted harm. One potential for harm from disposed waste lies in the migration of harmful constituents in the waste to the environment via water. This simple statement, when applied to the migration of a contaminant through and out of a monolithic form, gives rise to an interesting problem about the extreme short term leaching rates in a transport process defined solely by diffusion.

Consider a contaminated monolithic form, in particular a solid cylindrical shape of concrete embedded during mixing with a mobile species such as radioactive cesium, the leachate. Allowed to dry and cure, the cylinder is immersed in water, and the cesium leaches out in a manner that over the long term is consistent with a normal diffusion process with constant initial concentration and diffusion coefficient. Long term here is months and years. Our principle goal is to determine long-term behavior of the Cumulative Fraction Leached (CFL) with extreme short-term leach data; "extreme short-term" means days. We assume a given geometric structure of the waste form and the knowledge of an effective long-term diffusion coefficient for the leachate. However, for particular measured data, it became impossible to accurately model the leach rate over the extreme short term and long term combined.

Two explanations were plausible: The "pure" diffusion model mechanism for the leaching process was incorrect. Perhaps some other transport mechanism is at work. Alternatively, the constancy of the diffusion coefficient throughout the body or the constancy of the initial concentration, or both were in error. We address the alternative possibility. Indeed we hypothesize the following:

a. In a very thin boundary layer, about the thickness of the concrete backfill material, (i.e. sand) it is supposed that the diffusion coefficient is somewhat higher than that interior to the specimen.
b. The initial concentration of the radionuclide is greater in this boundary layer than in the interior where it is constant.

The physical reason for the first of these assumptions is that in the thin boundary layer the cement has less backfill material which is a total retardant to diffusion, making the effective diffusion higher there. The physical reasoning for the second assumption is more speculative. It is proposed that while the cement sets there is some rapid mobility of the species toward the boundary resulting in a higher concentration there. At this time magnetic resonance imaging equipment available to the authors cannot achieve the resolution necessary to confirm this assumption. As a point of interest, both assumptions, together with a thickness assumption for the boundary layer are needed to match the extreme short and long term shape of the Nomine [9] leach data.

Our model for the leaching process is based on a one dimensional diffusion equation of the form (1), on a general interval $[0, a]$, with the above assumptions built into $p(x)$ and $u_0(x)$. To compare results obtained with actual data the one dimensional data must be corrected by the surface/volume (S/V) ratio. With this done, and with the Assumptions a and b in effect, we obtain extremely accurate approximations to the data in Nomine [8] both in the short term and long. Study of the extreme short term leaching behavior requires very small time steps and this necessarily results in long computer runs to obtain accurate results (cf. Allen and Pitt [1]).

Naturally, it would be more desirable to determine the leach rates theoretically, and that is the intent of this paper. Denote by $u(x, t)$ the concentration of the leachant at position x and at time t. The total leachant remaining in the one dimensional specimen at time t is given by $\int_0^a u(x,t)\,dx$. The Cumulative Fraction Leached (CFL) by time t is given by

$$U(t) := \frac{\int_0^a u_0(x)\,dx - \int_0^a u(x,t)\,dx}{\int_0^a u_0(x)\,dx},$$

and collected data indicates that

$$\lim_{t \to 0^+} \frac{1}{\sqrt{t}} U(t)$$

should exist. Indeed, out main result yields a precise value for this limit.

By way of background, the total migration of waste from the storage facility to the groundwater supply is an enormously complex process that has been studied for at least twenty-five years and is still a hot topic today. It involves several independent and/or coupled processes, each of which is complex itself. Among these are water penetration into the facility (Ahn and Suzuki [2]), leaching from the waste form (Ahn and Suzuki [2]), deterioration of the container and deterioration of the solid phase (Matsuzuru and Suzuki [7]), migration through the backfill materials (Ahn and Suzuki [2]), structural integrity of the facility, and migration external to the facility to the groundwater supply (Lever, et al, [6]). We have determined two factors via the boundary layer hypothesis that are significant for finding a mathematical model that gives good approximations to actual data. These same factors have not been considered by other investigators (Godbee [5]; Matsuzuru and Ito [8]). Rather, these authors have concentrated on general theoretical solutions (usually of series type) of the diffusion equation based on a constant effective diffusion coefficient together with an empirical (mathematical) model which is then "tuned" to obtain good agreement with experimental results (Spence and Godbee, et al, [13]). The benchmark data with which we have compared our numerical results is the CEN-Saclay Long-Term Leach Data for the very mobile species cesium (Nomine, et al [9]). Various sized cylinders were used. All indicated very low long-term leach rates of 10^{-11} to 10^{-12} cm^2/sec. Unfortunately, these low leach rates were not observed until 30 to 60 days into the experiments and persisted for more than 700 days, would not have been so measured in standard short-term leach tests, such as ANSI 16.1 (ANSI/ANS 16.1, 1986).

1. MAIN RESULT

Suppose $p(x)$ is a smooth function on $[0,\pi]$ and there exists $p_1>0$ such that $p(x)\geq p_1$ for all $x\in[0,\pi]$. In addition, suppose $p(x)$ is symmetric about $x=\frac{\pi}{2}$. Let u_0 be a continuous function on $[0,\pi]$ such that if v_0 is the unique solution to

$$\left\{\begin{array}{l} -\frac{d}{dx}\left(p(x)v_0'(x)\right)=0,\ \ 0<x<\pi \\ v_0(0)=u_0(0),\ \ v_0(\pi)=u_0(\pi) \end{array}\right\} \tag{3}$$

then

$$u_0-v_0\in H^2\left((0,\pi),R\right)\cap H_0^1\left((0,\pi),R\right). \tag{4}$$

This is very little restriction on u_0. In fact, if $u_0\in H^2\left((0,1),R\right)$ then this will be satisfied.

We consider the diffusion equation

$$\left\{\begin{array}{l} u_t=\frac{\partial}{\partial x}\left(p(x)u_x\right),\ \ 0<x<\pi,\ \ t>0 \\ u(0,t)=u(\pi,t)=0,\ \ t>0 \\ u(x,0)=u_0(x),\ \ 0<x<\pi \end{array}\right\}. \tag{5}$$

Our primary goal is the following result.

Theorem 1.1. *Let $u(x,t)$ be the unique solution of (5). Then*

$$\lim_{t\to0^+}\frac{1}{\sqrt{t}}\int_0^\pi\left(u_0(x)-u(x,t)\right)dx=\frac{2\sqrt{p(0)}}{\sqrt{\pi}}\left(u_0(0)+u_0(\pi)\right).$$

Remark 1.1. *A simple change of variables can be used to verify that the result above remains the same if the interval $[0,\pi]$ is replaced with an arbitrary interval of the form $[0,a]$.*

We will need to recall some basic information to prove this result. First, if we denote the operator

$$A:D(A)\to L^2((0,\pi),R)$$

defined by

$$A(w)=\frac{d}{dx}\left(p(x)w_x\right)$$

for all

$$w\in D(A)=H^2\left((0,\pi),R\right)\cap H_0^1\left((0,\pi),R\right)$$

then A is the infinitesimal generator of a strongly continuous semi-group $\{T(t)\}_{t\geq 0}$ on L^2 (cf. Pazy [9]). As a result, from (4) we have

$$\lim_{h\to 0^+} \frac{(T(h)-I)(w_0)}{h} = A(w_0)$$

for all $w_0 \in D(A)$ (with the limit understood in the L^2 sense). Consequently,

$$\lim_{h\to 0^+} \frac{(T(h)-I)(u_0-v_0)}{h} = A(u_0-v_0). \tag{6}$$

Now, let

$$w_0 = u_0 - v_0$$

and suppose w is the unique solution of

$$\left\{ \begin{array}{l} w_t = \frac{\partial}{\partial x}(p(x)w_x), \;\; 0<x<\pi, \;\; t>0 \\ w(0,t) = w(\pi,t) = 0, \;\; t>0 \\ w(x,0) = w_0(x), \;\; 0<x<\pi \end{array} \right\}.$$

Then

$$w(x,t) = T(t)w_0.$$

Therefore,

$$\begin{aligned} \left| \frac{1}{\sqrt{t}} \int_0^\pi (w_0(x) - w(x,t))\, dx \right| &= \left| \sqrt{t} \frac{1}{t} \int_0^\pi (T(t)w_0 - w_0)\, dx \right| \\ &\leq \sqrt{t} \frac{\|T(t)w_0 - w_0\|_2}{t} \sqrt{\pi} \\ &\to 0 \text{ as } t \to 0^+ \end{aligned}$$

from (6). Let v be the solution to

$$\left\{ \begin{array}{l} v_t = \frac{\partial}{\partial x}(p(x)v_x), \;\; 0<x<\pi, \;\; t>0 \\ v(0,t) = v(\pi,t) = 0, \;\; t>0 \\ v(x,0) = v_0(x), \;\; 0<x<\pi \end{array} \right\}.$$

Then clearly

$$u = v + w.$$

So,

$$\frac{1}{\sqrt{t}} \int_0^\pi (u_0(x) - u(x,t))\, dx = \frac{1}{\sqrt{t}} \int_0^\pi (v_0(x) + w_0(x) - v(x,t) - w(t,x))\, dx$$

implying

$$\lim_{t\to 0^+} \frac{1}{\sqrt{t}} \int_0^\pi (u_0(x) - u(x,t))\, dx = \lim_{t\to 0^+} \frac{1}{\sqrt{t}} \int_0^\pi (v_0(x) - v(x,t))\, dx. \tag{7}$$

Consequently, we concentrate on the latter limit.

Let's start by writing $v(x,t)$ in terms of an eigenfunction expansion. Let $\{\lambda_n\}_{n=1}^\infty$ denote the eigenvalues of A listed in decreasing order. It is a simple matter to prove that each eigenvalue is negative and

$$-\lambda_n \geq p_1 n^2 \tag{8}$$

for every natural number n. In addition, if we let E_n denote the eigenspace associated with the eigenvalue λ_n, then

$$\dim(E_n) = 1.$$

It is well known (cf. Courant and Hilbert [2], p. 293 and 359) that these eigenspaces are orthogonal in $L^2\left((0,\pi),R\right)$ and

$$L^2\left((0,\pi),R\right)=\oplus_{n=1}^{\infty}E_n.$$

For each n let $\phi_n\in E_n$ such that $\|\phi_n\|_2=1$. Then $\{\phi_n\}_{n=1}^{\infty}$ is an orthonormal basis for $L^2\left((0,\pi),R\right)$. Also, from the properties of A, each of the ϕ_n is a smooth function. We can assume without loss of generality that these functions have been scaled such that

$$\phi_n'(0)>0$$

for each n.

We will make considerable use of the following classic results from Sturm-Liouville theory (cf. Courant and Hilbert [2], p. 336).

Theorem 1.2. *Let λ_n and ϕ_n be given as above and suppose that $p(x)$ is twice continuously differentiable on $[0,\pi]$. Define*

$$l=\int_0^{\pi}\frac{1}{\sqrt{p(x)}}dx.$$

Then

$$\lambda_n=-\frac{n^2\pi^2}{l^2}+O(1), \tag{9}$$

$$\phi_n(x)=\sqrt{\frac{2}{l}}\frac{\sin\left(n\frac{\pi}{l}\int_0^x\frac{1}{\sqrt{p(s)}}ds\right)}{\left(p(x)\right)^{1/4}}+O(\frac{1}{n}), \tag{10}$$

and

$$\phi_n'(x)=\sqrt{\frac{2}{l}}\frac{n\pi}{l}\frac{\cos\left(n\frac{\pi}{l}\int_0^x\frac{1}{\sqrt{p(s)}}ds\right)}{\left(p(x)\right)^{3/4}}+O(1). \tag{11}$$

Let $\langle\cdot,\cdot\rangle_2$ denote the L^2 inner product on $[0,\pi]$. Then we can write the eigenfunction expansion for $v(x,t)$ in the form

$$v(x,t)=\sum_{n=1}^{\infty}e^{\lambda_n t}\left\langle v_0,\phi_n\right\rangle_2\phi_n(x). \tag{12}$$

Furthermore, we can easily compute

$$\begin{aligned}\left\langle v_0,\phi_n\right\rangle_2&=\frac{1}{\lambda_n}\int_0^{\pi}v_0(x)\frac{d}{dx}\left(p(x)\phi_n'(x)\right)dx\\&=\frac{1}{\lambda_n}v_0(x)p(x)\phi_n'(x)|_{x=0}^{x=\pi}\end{aligned}$$

from (3). Consequently,

$$\left\langle v_0,\phi_n\right\rangle_2=\frac{p(0)}{\lambda_n}\left[u_0(\pi)\phi_n'(\pi)-u_0(0)\phi_n'(0)\right]$$

from the symmetry of $p(x)$. Similarly,

$$\left\langle 1,\phi_n\right\rangle_2=\frac{p(0)}{\lambda_n}\left[\phi_n'(\pi)-\phi_n'(0)\right].$$

Therefore, if we denote

$$a_n = (u_0(\pi)\phi_n'(\pi) - u_0(0)\phi_n'(0))\,(\phi_n'(\pi) - \phi_n'(0))$$

then

$$\frac{1}{\sqrt{t}}\int_0^{\pi} (v_0(x) - v(x,t))\,dx = \frac{1}{\sqrt{t}}\sum_{n=1}^{\infty}\left(1 - e^{\lambda_n t}\right)\frac{p(0)^2}{\lambda_n^2}a_n. \tag{13}$$

We will have use of the following results.

Lemma 1.3. *For each natural number n we have*

$$a_{2n-1} = \frac{4(2n-1)^2\pi^2}{l^3\,(p(0))^{3/2}}\,(u_0(\pi) + u_0(0)) + O(2n-1) \tag{14}$$

and

$$a_{2n} = O(1). \tag{15}$$

Proof. The result is a straight-forward calculation using the definition of a_k and (11). □

Lemma 1.4. *If $d > 0$ then*

$$\lim_{t\to 0^+}\sum_{n=1}^{\infty} e^{-d(2n-1)^2\pi^2h^2}h = \frac{1}{4\sqrt{\pi d}}. \tag{16}$$

Proof. Note that for each $h > 0$, the sum

$$\sum_{n=1}^{\infty} e^{-d(2n-1)^2\pi^2h^2}\,(2h)$$

is the approximation of the integral

$$\int_0^{\infty} e^{-d\pi^2x^2}dx = \frac{1}{2\sqrt{\pi d}}$$

via the midpoint method. The result follows. □

We are now in a position to prove our main result.

Proof. (of our main result) It is a simple matter to prove that (9), (11), (14) and (15) imply we can apply l'Hopital's rule to obtain

$$\lim_{t\to 0^+}\frac{1}{\sqrt{t}}\sum_{n=1}^{\infty}\left(1 - e^{\lambda_n t}\right)\frac{p(0)^2}{\lambda_n^2}a_n = \lim_{t\to 0^+}2\sqrt{t}\sum_{n=1}^{\infty}e^{\lambda_n t}\frac{p(0)^2}{(-\lambda_n)}a_n.$$

Therefore, from (13) we have

$$\begin{aligned}\lim_{t\to 0^+}\frac{1}{\sqrt{t}}\int_0^{\pi}(v_0(x) - v(x,t))\,dx &= 2\lim_{t\to 0^+}\sqrt{t}\sum_{n=1}^{\infty}e^{\lambda_n t}\frac{p(0)^2}{(-\lambda_n)}a_n \\ &= 2\lim_{h\to 0^+}\sum_{n=1}^{\infty}e^{\lambda_n h^2}h\frac{p(0)^2}{(-\lambda_n)}a_n \qquad (17)\end{aligned}$$

(provided the latter limit exists). Set

$$f(h) = \frac{2}{(u_0(\pi) + u_0(0))}\sum_{n=1}^{\infty}e^{\lambda_{2n-1}h^2}h\frac{1}{(-\lambda_{2n-1})}a_{2n-1}$$

and

$$g(h) = \sum_{n=1}^{\infty} e^{\lambda_{2n} h^2} h \frac{p(0)^2}{(-\lambda_{2n})} a_{2n}.$$

If we apply (8), (15) and (16) then it follows that

$$\lim_{h \to 0^+} g(h) = 0. \tag{18}$$

Also, note that from (9), (11) and (14) we have

$$\frac{a_{2n-1}}{(-\lambda_{2n-1})} = \frac{4}{l\,(p(0))^{3/2}} \left(u_0(\pi) + u_0(0)\right) + O\left(\frac{1}{n}\right).$$

Consequently,

$$f(h) = \sum_{n=1}^{\infty} e^{\lambda_{2n-1} h^2} h \left(\frac{8}{l\,(p(0))^{3/2}} + O\left(\frac{1}{n}\right) \right).$$

Easily,

$$\sum_{n=1}^{\infty} e^{\lambda_{2n-1} h^2} h O\left(\frac{1}{n}\right) \to 0$$

as $h \to 0^+$ (just apply (16)). Now set

$$d = \frac{1}{l^2}.$$

Then

$$\left| \sum_{n=1}^{\infty} e^{\lambda_{2n-1} h^2} h - \sum_{n=1}^{\infty} e^{-d(2n-1)^2 \pi^2 h^2} h \right| = \left| \sum_{n=1}^{\infty} \left(e^{\lambda_{2n-1} h^2} - e^{-d(2n-1)^2 \pi^2 h^2} \right) h \right|.$$

Note that if $0 < y < z$ then

$$\left| e^{-y} - e^{-z} \right| \le e^{-y} \left| y - z \right|.$$

Also, from (8) we know there exists $\varepsilon > 0$ such that

$$\varepsilon \le d$$

and

$$\varepsilon (2n-1)^2 \pi^2 \le \lambda_{2n-1} \text{ for all } n \ge M.$$

(in fact, $\varepsilon = p_1$ works). As a result,

$$\begin{aligned} \left| \sum_{n=1}^{\infty} \left(e^{\lambda_{2n-1} h^2} - e^{-d(2n-1)^2 \pi^2 h^2} \right) h \right| &\le \sum_{n=1}^{\infty} e^{-\varepsilon (2n-1)^2 \pi^2 h^2} \left| \lambda_{2n-1} + d(2n-1)^2 \pi^2 \right| h^3 \\ &\le K \sum_{n=1}^{\infty} e^{-\varepsilon (2n-1)^2 \pi^2 h^2} h^3 \end{aligned}$$

for some $K > 0$, from (9). However, from (16) this last term goes to zero as $h \to 0^+$. Therefore,

$$\begin{aligned}
\lim_{h\to 0^+} f(h) &= \frac{8}{l\,(p(0))^{3/2}} \lim_{h\to 0^+} \sum_{n=M}^{\infty} e^{\lambda_{2n-1}h^2} h \\
&= \frac{8}{l\,(p(0))^{3/2}} \lim_{h\to 0^+} \sum_{n=M}^{\infty} e^{-d(2n-1)^2\pi^2h^2} h \\
&= \frac{8}{l\,(p(0))^{3/2}} \lim_{h\to 0^+} \sum_{n=1}^{\infty} e^{-d(2n-1)^2\pi^2h^2} h \\
&= \frac{8}{l\,(p(0))^{3/2}} \frac{1}{4\sqrt{\pi d}} \\
&= \frac{8}{4\sqrt{\pi}\,(p(0))^{3/2}} \qquad (19)
\end{aligned}$$

from (16) and the definition of d. Finally, therefore, if we combine (7), (17), the definitions of $f(h)$ and $g(h)$, (18) and (19) then we have

$$\begin{aligned}
\lim_{t\to 0^+} \frac{1}{\sqrt{t}} \int_0^{\pi} (v_0(x) - v(x,t))\,dx &= \frac{8}{4\sqrt{\pi}\,(p(0))^{3/2}} (p(0))^2 \left(u_0(\pi) + u_0(0)\right) \\
&= \frac{2\sqrt{p(0)}}{\sqrt{\pi}} \left(u_0(\pi) + u_0(0)\right). \quad \square
\end{aligned}$$

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