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Finite Transition Times for Diffusion-Decay Problems

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Abstract

When a system progresses from its initial condition to its steady-state, the duration of this transition takes, mathematically, an infinitely long time period. In the context of practical uses, like science and engineering, it is useful to consider a *finite* transition time at which there is only an arbitrary distinction between the transient solution at that time and the steady-state. In this report, we extend a method for finding the finite transition time for homogeneous diffusion problems to the case of systems governed by diffusion-decay. The extended finite transition time formula retains the properties of the homogeneous method that allows it to determine a time to steady-state without having to calculate the transient solution of the underlying partial differential equation. The results demonstrate that the procedure is accurate to a remarkably high degree for increasing index k, and also that the estimate is reasonably accurate as a rule-of-thumb approximation for indices as small as $k = 2$. The development of this procedure then lends itself to future extension into problems such as coupled linear diffusion problems, which - when uncoupled into two diffusion-decay problems - can be solved using the procedure outlined in this report.

1 Introduction

When physical systems that are governed by diffusive processes undergo sudden changes in their boundary conditions, they asymptotically approach their new equilibrium states over an infinite time period (McNabb & Wake 1991). While this is true in a mathematical sense, it is useful in a scientific and engineering context to consider when a system is only nominally distinguishable from its steady-state. By utilising a finite time period after which this arbitrary closeness is met, a practical and useful answer to the question of the time to equilibrium is achieved.

Recently, Carr (2017) presented a method through which these *finite transition times* can be calculated for a linear, homogeneous diffusion equation, which has the advantage of avoiding having to calculate the transient solution of the problem. In this report, we aim to extend Carr's method to diffusion-decay and associated coupled linear diffusion problems. Mathematical models that utilise these models are widely used in science and engineering disciplines, contexts that benefit from the establishment of a finite transition time, such as convective drying of materials (e.g. Barati & Esfahani (2012)).

We define the distinction between a local and a global transition time as follows. A local transition time is the finite estimate of time for the solution to the governing equation $u(x,t)$ to transition from its initial condition $u_0(x)$ to its steady-state solution (which we denote $u_\infty(x)$) at some position x in the system domain $\mathcal{L} = (l_0, l_m)$. Conversely, the global transition time is an estimate for how long it

takes for the entire system to reach its steady-state. Below, we establish mathematical definitions for these concepts as in Carr (2017):

Definition 1.1. (Local transition time) The local transition time, $t_s(x)$, is the transition time evaluated as a function of the position $x \in \mathcal{L}$ and $u(x,0) \neq u_\infty(x)$. The local transition time is defined as some value for $t > 0$ that satisfies

$$\frac{u(x,t) - u_\infty(x)}{u_0(x) - u_\infty(x)} = \delta, \tag{1}$$

where $0 < \delta \ll 1$.

The choice of δ can be made according to appropriate conditions of the physical problem being considered, which is a significant advantage of the method outlined in Carr (2017).

Definition 1.2. (Global transition time) The global transition time is defined as the supremum of the local finite transition time,

$$\hat{t}_s \coloneqq \sup_{x \in \mathcal{L}} \left(t_s(x) \right), \tag{2}$$

and the supremum is taken across the system domain (the domain of $t_s(x)$).

Next, we can define a function $F(t;x)$, analogous with probability theory (Ellery et al. 2012), such that

$$F(t;x) \coloneqq 1 - \frac{u(x,t) - u_\infty(x)}{u_0(x) - u_\infty(x)}. \tag{3}$$

Notably, $F(t;x)$ satisfies the properties of a cumulative distribution function, in that (i) $F(0;x) = 0$, (ii) $\lim_{t\to\infty} F(t;x) = 1$, and (iii) $F(t;x)$ is monotonic. The condition (iii) is developed from the assumption that on $x \in \mathcal{L}$, $u(x,t)$ monotonically increases if $u_0(x) < u_\infty(x)$ and monotonically decreases if $u_0(x) > u_\infty(x)$ (see Carr (2017)). Using Definition 1.1 in (3), we can also define the transition time as the value of $t > 0$ satisfying $F(t;x) = 1 - \delta$. These properties can be seen in Figure 1.

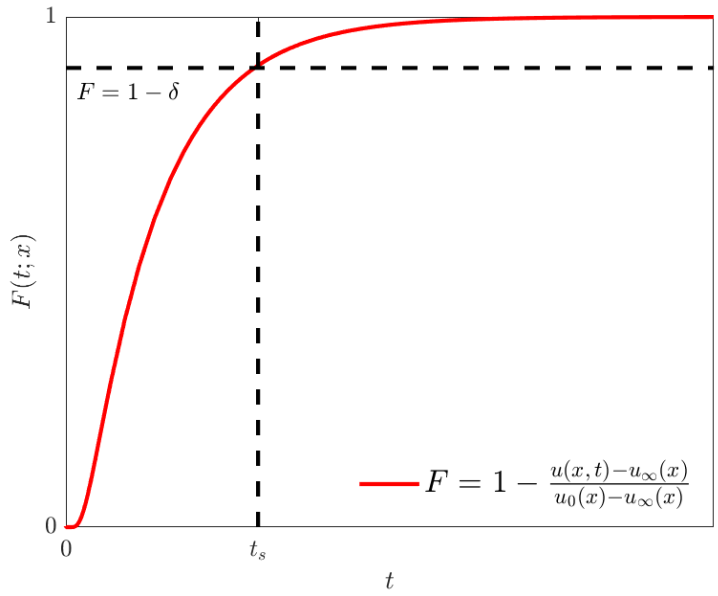

Figure 1: The defined function $F(t;x)$ at some position x, clearly demonstrating that $F(t;x)$ meets the requirements of a cumulative distribution function. Definition 1.1 along with (3) means that when $F(t;x) = 1-\delta$, then $t = t_s$.

Next, the k-th moment at position x can be defined as:

$$M_k(x) \coloneqq \int_0^\infty t^k f(t;x)\, dt, \tag{4}$$

where differentiating (3) with respect to t yields the associated probability density function (Simpson 2018):

$$f(t;x) = \frac{1}{u_\infty(x) - u_0(x)} \frac{\partial}{\partial t} \left(u(x,t) - u_\infty(x)\right). \tag{5}$$

Carr's method for determining the moments and transition time utilises the definition in Equation (4) to determine a precise estimate for the transition time $\hat{t}_s$ for some corresponding δ. In this report where we extend this method, we will also use this definition in a similar approach.

Statement of Authorship

- Jonah Klowss developed the MATLAB code and extensions to the finite transition time method, produced the results, interpreted the data, and wrote this report.
- Elliot Carr provided guidance through the project, proposed the extension to the homogenous diffusion problem, supervised the work, and proofread this report.

2 Diffusion-decay model

The model used in this report is described as follows. The governing equation is the diffusion-decay equation

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} - \kappa u, \tag{6a}$$

on the interval $x \in (l_0, l_m)$ for $t > 0$, with the boundary conditions

$$a_L u(l_0, t) - b_L \frac{\partial u}{\partial x}(l_0, t) = c_L, \tag{6b}$$

$$a_R u(l_m, t) + b_R \frac{\partial u}{\partial x}(l_m, t) = c_R, \tag{6c}$$

and the initial condition on $x \in (l_0, l_m)$,

$$u(x, 0) = u_0(x). \tag{6d}$$

The solution $u(x, t)$ is the quantity in question (e.g. concentration, temperature) at the position x and time t. The initial condition $u_0(x)$ is specified for the problem, and the parameters $D > 0$ and $\kappa > 0$ are the diffusion coefficient and decay constant respectively.

The diffusion-decay model in (6) also has an associated steady-state solution $u_\infty(x)$, which satisfies:

$$Du''_\infty(x) - \kappa u_\infty = 0, \tag{7a}$$

$$a_L u_\infty(l_0) - b_L u'_\infty(l_0) = c_L, \tag{7b}$$

$$a_R u_\infty(l_o) + b_R u'_\infty(l_m) = c_R. \tag{7c}$$

3 Moment computation

Notably, the definition of the moments in Equation (4) contains an explicit expression for the solution $u(x, t)$. In this section, we extend Carr's method for calculating the first q moments (specifically $M_k(x)$, $k = 1, ..., q$) to the diffusion-decay problem. Combining the equations (4) and (5) yields an equivalent expression for $M_k(x)$:

$$M_k(x) = \frac{1}{h(x)} \int_0^\infty t^k \frac{\partial}{\partial t} \left(u(x, t) - u_\infty(x)\right) dt, \tag{8}$$

where $h(x) \coloneqq u_\infty(x) - u_0(x)$. Integrating by parts and observing that – by definition – $\lim_{t\to\infty} u(x,t) = u_\infty(x)$, then it follows that $\lim_{t\to\infty} t^k \left(u(x,t) - u_\infty(x)\right) = 0$. This also relies on $u(x,t)$ tending to $u_\infty(x)$ exponentially, and faster than t^k tending to infinity. Hence,

$$M_k(x) = \frac{k}{h(x)} \int_0^\infty t^{k-1} \left[u_\infty(x) - u(x,t)\right] \, dt, \tag{9}$$

The method described in Carr (2017) has the advantage in that it does not require computation of the transient solution, avoiding this by determining a boundary value problem for the k-th moment. In this project, we aim to achieve the same goal, starting by defining $\overline{M}_k(x) \coloneqq M_k(x)h(x)$. Then:

$$\overline{M}_k(x) = k \int_0^\infty t^{k-1} \left[u_\infty(x) - u(x,t)\right] \, dt. \tag{10}$$

Considering the second derivative of this expression with respect to x,

$$\overline{M}_k''(x) = k \int_0^\infty t^{k-1} \left[u_\infty''(x) - \frac{\partial^2 u}{\partial x^2}(x,t)\right] \, dt, \tag{11}$$

and recalling the governing equation of the model (6a) and its associated steady-state problem (7a), then Equation (11) becomes

$$\overline{M}_k''(x) = k \int_0^\infty t^{k-1} \left[\frac{\kappa}{D} u_\infty(x) + \frac{\partial}{\partial t}\left(\frac{u_\infty(x)}{D}\right) - \frac{1}{D}\frac{\partial u}{\partial t}(x,t) - \frac{\kappa}{D} u(x,t)\right] \, dt. \tag{12}$$

Rearranging the terms into a more useful form,

$$\overline{M}_k''(x) = \frac{\kappa}{D}\left(k \int_0^\infty t^{k-1} \left[u_\infty(x) - u(x,t)\right] \, dt\right) - \frac{k}{D}\left(\int_0^\infty t^{k-1} \frac{\partial}{\partial t}\left[u(x,t) - u_\infty(x)\right] \, dt\right), \tag{13}$$

it is clear that the left bracket is $\overline{M}_k(x)$ from (10), and the right bracket is the $(k-1)$-th scaled moment $\overline{M}_{k-1}(x)$ from (8). Hence, a boundary value problem for $\overline{M}_k(x)$ is derived:

$$\overline{M}_k''(x) = \frac{\kappa}{D}\overline{M}_k(x) - \frac{k}{D}\overline{M}_{k-1}(x), \tag{14a}$$

$$a_L \overline{M}_k(l_0) - b_L \overline{M}_k'(l_0) = 0, \tag{14b}$$

$$a_R \overline{M}_k(l_m) + b_R \overline{M}_k'(l_m) = 0, \tag{14c}$$

where the boundary conditions in (14b) and (14c) are determined by using the definitions of the moments and the boundary conditions of the original problem (6b) and (6c). Critically, this boundary

value problem allows us to compute the moments without the transient solution.

3.1 Solving the ODE

The solution to the ODE (14a) starts with the homogeneous problem $\overline{M}_k''(x) - \frac{\kappa}{D}\overline{M}_k(x) = 0$, which solves to give a fundamental set of solutions $F = \left\{ e^{\sqrt{\kappa/D}\,x},\, e^{-\sqrt{\kappa/D}\,x} \right\}$. Consequently, $\overline{M}_k(x)$ takes the form:

$$\overline{M}_k(x) = c_{k,1}e^{\sqrt{\kappa/D}\,x} + c_{k,2}e^{-\sqrt{\kappa/D}\,x} + G_k(x), \tag{15}$$

with $G_k(x)$ being the particular solution. To solve for $G_k(x)$ we employ Cramer's method for variation of parameters, since this is the approach best suited to the iterative nature of the problem and the (most often) unknown nature of $\overline{M}_{k-1}(x)$. As a result, the particular solution is

$$G_k(x) = \varphi_k(x)e^{\sqrt{\kappa/D}\,x} + \psi_k(x)e^{-\sqrt{\kappa/D}\,x}, \tag{16}$$

where the functions $\varphi_k(x)$ and $\psi_k(x)$ are determined by integrating their derivatives, which are devised from Cramer's rule:

$$\varphi_k'(x) = \frac{\Delta_1}{|W|}, \tag{17}$$

$$\psi_k'(x) = \frac{\Delta_2}{|W|}. \tag{18}$$

The values Δ_1, Δ_2, and $|W|$ are determinants of the associated matrices, W being the Wronskian, such that:

$$|W| = \begin{vmatrix} e^{\sqrt{\kappa/D}\,x} & e^{-\sqrt{\kappa/D}\,x} \\ \sqrt{\frac{\kappa}{D}}e^{\sqrt{\kappa/D}\,x} & -\sqrt{\frac{\kappa}{D}}e^{-\sqrt{\kappa/D}\,x} \end{vmatrix}, \tag{19}$$

$$\Delta_1 = \begin{vmatrix} 0 & e^{-\sqrt{\kappa/D}\,x} \\ -\frac{k}{D}\overline{M}_{k-1}(x) & -\sqrt{\frac{\kappa}{D}}e^{-\sqrt{\kappa/D}\,x} \end{vmatrix} = \frac{k}{D}\overline{M}_{k-1}(x)e^{-\sqrt{\kappa/D}\,x}, \tag{20}$$

$$\Delta_2 = \begin{vmatrix} e^{\sqrt{\kappa/D}\,x} & 0 \\ \sqrt{\frac{\kappa}{D}}e^{\sqrt{\kappa/D}\,x} & -\frac{k}{D}\overline{M}_{k-1}(x) \end{vmatrix} = -\frac{k}{D}\overline{M}_{k-1}(x)e^{\sqrt{\kappa/D}\,x}. \tag{21}$$

With this in mind, the constants $c_{k,1}$ and $c_{k,2}$ are now determined by substituting (15) into the boundary conditions (14b) and (14c). This results in a linear system,

$$\mathbf{Ac} = \mathbf{b}, \tag{22}$$

with $\mathbf{c} = [c_{k,1},\, c_{k,2}]^T$, and

$$\mathbf{A} = \begin{pmatrix} a_L e^{\sqrt{\kappa/D}\, l_0} - b_L\sqrt{\frac{\kappa}{D}} e^{\sqrt{\kappa/D}\, l_0} & a_L e^{-\sqrt{\kappa/D}\, l_0} + b_L\sqrt{\frac{\kappa}{D}} e^{-\sqrt{\kappa/D}\, l_0} \\ a_R e^{\sqrt{\kappa/D}\, l_m} + b_R\sqrt{\frac{\kappa}{D}} e^{\sqrt{\kappa/D}\, l_m} & a_R e^{-\sqrt{\kappa/D}\, l_m} - b_R\sqrt{\frac{\kappa}{D}} e^{-\sqrt{\kappa/D}\, l_m} \end{pmatrix}, \tag{23}$$

$$\mathbf{b} = \begin{pmatrix} b_L G_k'(l_0) - a_L G_k(l_0) \\ -b_R G_k'(l_m) - a_R G_k(l_m) \end{pmatrix}. \tag{24}$$

In the case of homogeneous Neumann boundary conditions at both ends, the solution would likely require an additional constraint to be applied to the system (Carr & Turner 2016). We do not consider this case in any examples in this report.

Once the values of $c_{k,1}$ and $c_{k,2}$ are determined, and subsequently an expression for $\overline{M}_k(x)$ is found, then the k-th moment is calculated according to $M_k(x) = \dfrac{1}{h(x)}\overline{M}_k(x)$. The procedure outlined in this section is summarised in Algorithm 1:

Algorithm 1: Computation of diffusion-decay moments

$\overline{M}_0(x) = u_\infty(x) - u_0(x)$
for $k = 1, ..., q$
  $\Delta_1 = \dfrac{k}{D}\overline{M}_{k-1}(x) e^{-\sqrt{\kappa/D}\, x}$
  $\Delta_2 = -\dfrac{k}{D}\overline{M}_{k-1}(x) e^{\sqrt{\kappa/D}\, x}$
  $\varphi_k(x) = \displaystyle\int_0^\infty \frac{\Delta_1}{|W|}\, dx$
  $\psi_k(x) = \displaystyle\int_0^\infty \frac{\Delta_2}{|W|}\, dx$
  $G_k(x) = \varphi_k(x) e^{\sqrt{\kappa/D}\, x} + \psi_k(x) e^{-\sqrt{\kappa/D}\, x}$
  Compute $c_{k,1}$ and $c_{k,2}$ from $\mathbf{Ac} = \mathbf{b}$
  $\overline{M}_k(x) = c_{k,1} e^{\sqrt{\kappa/D}\, x} + c_{k,2} e^{-\sqrt{\kappa/D}\, x} + G_k(x)$
  $M_k(x) = \overline{M}_k(x)/\overline{M}_0(x)$
end

Notably, the 0-th moment $M_0(x) = 1$, and so $\overline{M}_0(x) = h(x)$, making it a useful substitute in the algorithm when calculating the k-th moment from its scaled counterpart.

4 Estimates of Transition Time

The transition time estimate formula derived by Carr (2017) remains much the same for the diffusion-decay problem (6). The analytical solution for this problem takes the form,

$$u(x,t) = u_\infty(x) + \sum_{n=1}^{\infty} \gamma_n(x) e^{-(\lambda_n+\kappa)t}. \tag{25}$$

This functional form is essentially identical to the analytical solution to the homogeneous diffusion problem,

$$u_h(x,t) = u_\infty(x) + \sum_{n=1}^{\infty} \gamma_n(x) e^{-t\xi_n}, \tag{26}$$

particularly when taking a choice of $\xi_n = \lambda_n + \kappa$. Substituting (25) into (3), then the cumulative distribution $F(t;x)$ takes the form

$$F(t;x) = 1 - \sum_{n=1}^{\infty} \zeta_n(x) e^{-t\xi_n}, \tag{27}$$

where $\zeta_n(x) = \gamma_n(x)/[u_0(x) - u_\infty(x)]$. Assuming, without loss of generality, that the ξ_i are denoted in ascending order such that $\xi_1 < \xi_2 < ...$, and $\zeta_1(x) \neq 0$ (see Carr (2017)), then an asymptotic approximation for the cumulative distribution function is reached:

$$F(t;x) \sim 1 - \zeta_1(x) e^{-t\xi_1}, \qquad \text{as } t \to \infty. \tag{28}$$

If approximating the behaviour of $F(t;x)$ for large t, it follows then that the below form is appropriate:

$$F(t;x) \simeq 1 - \alpha(x) e^{-t\beta(x)}, \tag{29}$$

where the functions $\alpha(x)$ and $\beta(x)$ are both unknown thus far. Recalling the other definition of the cumulative distribution function in (3) and invoking Definition 1.1, then the finite transition time is the value of $t > 0$ such that $F(t;x) = 1 - \delta$. Equating this expression with (29), then solving for t gives an expression of the local transition time as a function of position x (Carr 2017),

$$t_s(x) = \frac{1}{\beta(x)} \ln\left(\frac{\alpha(x)}{\delta}\right). \tag{30}$$

4.1 Determining the unknown functions

We follow the method in Carr (2017) to find the unknown functions $\alpha(x)$ and $\beta(x)$, which (30) shows are useful for determining an expression for the finite transition times. Differentiation of the cumulative distribution function of the form in (27) gives its associated probability density function,

$$f(t;x) = \sum_{n=1}^{\infty} \zeta_n(x)\xi_n e^{-t\xi_n}. \tag{31}$$

Substituting this form into the moment definition in (4), an expression for $M_k(x)$ is found:

$$M_k(x) = k! \sum_{n=1}^{\infty} \frac{\zeta_n}{\xi_n^k}. \tag{32}$$

Because $\xi_1 < \xi_n$, for $n = 2, 3, ...$, then terms with smaller ξ will dominate, and so $M_k(x)$ is asymptotically determined by

$$M_k(x) \sim \frac{\zeta_1 k!}{\xi_1^k}, \qquad \text{as } k \to \infty. \tag{33}$$

The observation in (33), along with the relation between ζ_1, ξ_1, $\alpha(x)$, and $\beta(x)$ from (28) and (29), gives the pair of coupled equations for the $(k-1)$-th and k-th moments below:

$$\frac{\alpha(x)}{\beta(x)^{k-1}} = \frac{M_{k-1}(x)}{(k-1)!},$$
$$\frac{\alpha(x)}{\beta(x)^{k}} = \frac{M_{k}(x)}{k!}.$$

Solving this system of equations yields expressions for $\alpha_k(x)$ and $\beta_k(x)$, which are now dependent on the $(k-1)$-th and k-th moments:

$$\alpha_k(x) = \frac{M_k(x)}{k!}\left(\frac{kM_{k-1}(x)}{M_k(x)}\right)^k,$$
$$\beta_k(x) = \frac{kM_{k-1}(x)}{M_k(x)}.$$

Hence, we can insert these expressions into (30),

$$t_s(x) = \frac{M_k(x)}{kM_{k-1}(x)} \ln\left[\frac{M_k(x)}{k!\delta}\left(\frac{kM_{k-1}(x)}{M_k(x)}\right)^k\right], \tag{34}$$

thereby determining an estimate for the finite transition time as a function of x, dependent on the k-th moments. Since, as shown in Section 3, the transient solution is not needed to calculate the k-th

moment, then so too can the finite transition time be determined without the use of the transient solution itself. Additionally, due to the asymptotic relationships in (28) and (33), we expect this estimate to be more accurate for larger values of k. This will be assessed further in Section 5. This result is the same as the one found in Carr (2017), so the expression for the transition time is not changed in the adaptation from homogeneous diffusion to diffusion-decay.

5 Results

To assess the accuracy of this method, we look at two different example cases. Case A has a Dirichlet condition on the left boundary, and a Neumann condition on its right boundary. Case B has two Neumann conditions, one homogeneous and one non-homogeneous. We describe each case as follows:

Case A.	*Case B.*
$u(0,t)=1, \quad \dfrac{\partial u}{\partial x}(1,t)=0$	$u(0,t)-0.1\dfrac{\partial u}{\partial x}(x,t)=0, \quad u(1,t)=0.5$
$D=1,\ \kappa=0.75, \quad u(x,0)=0$	$D=0.01,\ \kappa=0.03, \quad u(x,0)=1$

In each case, the domain of the system is $\mathcal{L}=[0,1]$. Importantly, both cases meet the requirements for the cumulative distribution function established in Section 1; namely the monotonic increase of $F(t;x)$, due to the monotonic increase of $u(x,t)$ toward $u_\infty(x)$ for all $x \in \mathcal{L}$. The choices of the diffusion constant D and the decay parameter κ are made so that the decay is not so insignificant as to have a negligible effect, but not so large as to dominate over the diffusion.

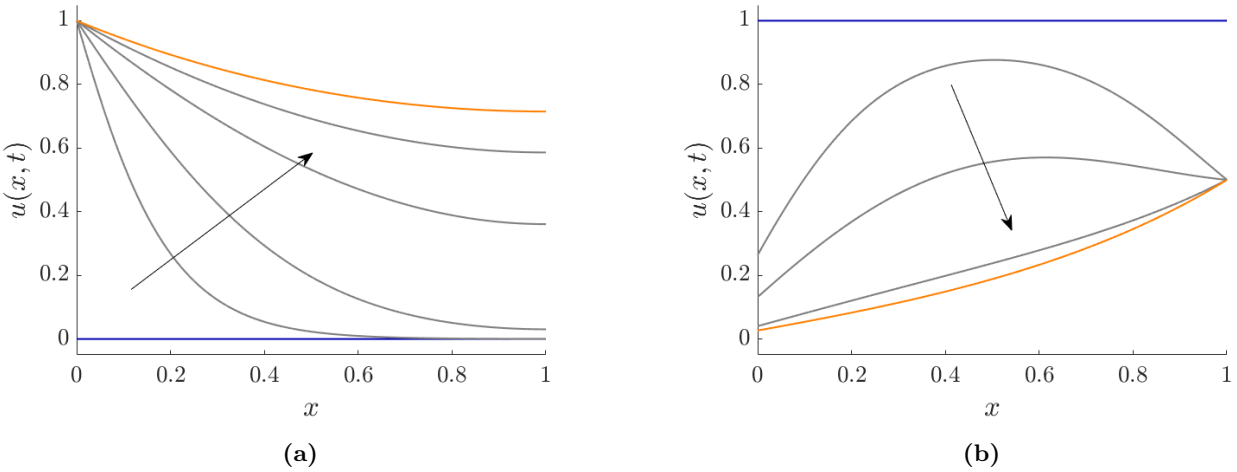

Figure 2: Plot of $u(x,t)$ for (a) Case A, and (b) Case B, where the arrow indicates the behaviour with increasing time, and blue and yellow are the initial and steady-state solutions of the system respectively. For Case A, the grey lines are plotted at $t=0.02$, 0.08, 0.32 and 0.64, and Case B has its lines plotted at $t=3$, 9, and 27.

Figure 2 shows the progression of the systems from their initial condition (blue) to their steady-states (yellow). The grey lines that indicate the progression to the steady-state along the direction of the arrow are placed at exponentially increasing time intervals, indicating that with increasing t, the duration requirement to make an approximately similar progression toward the steady state is longer.

In Table 1 we demonstrate the effect of increasing k in comparison with the result for the finite transition time determined from Definitions 1.1 and 1.2. For Case A, the analytical solution present in these definitions is taken from the first 100 terms of the eigenfunction expansion, which is then solved for $\hat{t}_s$. The "exact" transition time for Case B is taken by spatially discretising the system, and solving the resulting ODE with MATLAB's `ODE15S` function (Mathworks 2019).

Table 1: Comparisons between the analytically solved transition time, $\hat{t}_s$, and the global transition time estimates $\hat{t}_s^{(k)}$ with moment indices k. Different tolerances δ of 0.10, 0.05, 0.02, and 0.01 are considered.

	$\hat{t}_s^{(k)}$	k	$\delta = 0.10$	$\delta = 0.05$	$\delta = 0.02$	$\delta = 0.01$
Case A	$\hat{t}_s^{(1)}$	$k = 1$	0.9297	1.2096	1.5796	1.8594
	$\hat{t}_s^{(2)}$	$k = 2$	0.8178	1.0427	1.3398	1.5646
	$\hat{t}_s^{(5)}$	$k = 5$	0.8125	1.0280	1.3128	1.5283
	$\hat{t}_s^{(10)}$	$k = 10$	0.8126	1.0281	1.3128	1.5283
	$\hat{t}_s^{(15)}$	$k = 15$	0.8126	1.0281	1.3128	1.5283
	$\hat{t}_s$		0.8126	1.0281	1.3128	1.5283
Case B	$\hat{t}_s^{(1)}$	$k = 1$	24.5897	31.9919	41.7772	49.1794
	$\hat{t}_s^{(2)}$	$k = 2$	22.6026	29.0022	37.4619	43.8614
	$\hat{t}_s^{(5)}$	$k = 5$	22.5220	28.7512	36.9023	43.0955
	$\hat{t}_s^{(10)}$	$k = 10$	22.5298	28.7212	36.9057	43.0970
	$\hat{t}_s^{(15)}$	$k = 15$	22.5299	28.7212	36.9057	43.0970
	$\hat{t}_s$		22.5290	28.7212	36.9059	43.0973

Case A and Case B both demonstrate highly accurate estimates for the actual, analytical transition time values. In all combinations of Case A or B and a choice of δ, the choice of $k = 1$ causes a small overestimate for the transition time. Increasing the iteration count by just one index to $k = 2$ allows for a dramatic decrease in the error of the procedure, and by $k = 5$ the estimates for Case A are either very close, or equal, to the analytical solution to four digits of precision.

Case B has some more interesting results, in that it takes longer for the transition time estimate to reach this level of accuracy (approximately 10 iterations of k). Some discrepancy between the actual transition time and that derived from the moments can reasonably be explained by the inherent error

present from the spatial discretisation process. Despite this error, the estimates of the transition time are highly accurate to an order of magnitude that allows them to be reasonable estimates in their appropriate applications.

Also, we may observe an increase in error associated with estimates of the finite transition time for larger values of δ. This is because as δ is increased, the "at steady state" condition is closer to the initial condition, and so the system reaches this point faster. The consequence of this is that t_s is smaller, and for large δ this acts in contrast to the aim of making the large-time asymptotic approximation in (28). Thus, for smaller t, this relation is less reliable and so we expect a more pronounced error.

The values of the transition time estimate with increasing k do resemble an asymptotic progression toward a final quantity, both in the behaviour described earlier with the immediate increase in accuracy with just one iteration, and also in the slowing approach with higher order iterations as they begin to settle toward the final value. Looking at the transition time estimate for Case A with $\delta = 0.01$, and considering all $k = 1, ..., 15$, we can observe this effect in Figure 3 as confirmation of the asymptotic relation in (33).

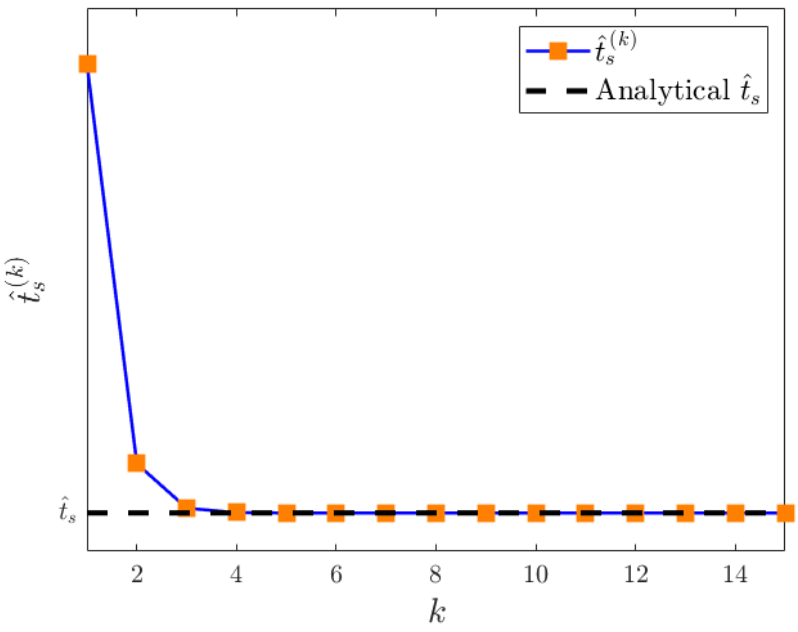

Figure 3: Plot of the transition time estimate $\hat{t}_s^{(k)}$, showing the accuracy of the asymptotic approximation in (33) increasing with higher order values of k.

The advantage of Carr's method is that it allows for the selection of two parameters – δ and k – that can be of a choice that is suitable for various applications. The use of δ allows for the closeness

to steady-state to be chosen based on the specific physical constraints or behaviours of a system. Similarly, choices of larger k allow for a more precise determination of the transition time with the expected consequence of increased computational cost. Choosing lower values of k may be more practical for some uses where constraints on the available computation time are present, and the quick convergence evident from the values in Table 1 and Figure 3 demonstrate that such a compromise may be worthwhile when necessary.

6 Conclusions

In summary, we have extended Carr's method from a diffusion-only problem to a diffusion-decay problem. As with the diffusion-only case, the diffusion-decay formula for the finite transition time does not require a calculation of the transient solution itself, depending instead on calculating the moments through an iterative process, while remaining tied to the original problem by using its boundary conditions. In addition, the transition time formula allows for flexibility regarding the choices of its parameters δ and k, which may have intuitive choices depending on the constraints or physical properties of the system that is being considered.

The results show that the accuracy of a choice of $k = 2$ is quite significant and lends itself well to being a quick, reasonable estimate of the transition time without having to commit to the calculation of even more higher-order moments. The overall accuracy of this approach is reasonably high, and so the extended method allows for calculations of transition times for systems that are governed by diffusion-decay.

Furthermore, this extension allows for the possibility of exploring coupled linear diffusion problems, and how it may be possible to determine the transition time to the steady-states of the two species present. If possible, reducing these problems into diffusion-decay problems could allow for the use of the algorithm and approach outlined in this report, and by extension the development of a procedure through which a transition time estimate for a coupled diffusion problem could be achieved. There are multiple avenues through which an approach to the solution of this problem may be taken, which can be investigated in future works.

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