# Critical time scales for advection-diffusion-reaction processes

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The concept of local accumulation time (LAT) was introduced by Berezhkovskii and co-workers to give a finite measure of the time required for the transient solution of a reaction-diffusion equation to approach the steady-state solution [A. M. Berezhkovskii, C. Sample, and S. Y. Shvartsman, Biophys. J. **99**, L59 (2010); Phys. Rev. E **83**, 051906 (2011)]. Such a measure is referred to as a critical time. Here, we show that LAT is, in fact, identical to the concept of mean action time (MAT) that was first introduced by McNabb [A. McNabb and G. C. Wake, IMA J. Appl. Math. **47**, 193 (1991)]. Although McNabb's initial argument was motivated by considering the mean particle lifetime (MPLT) for a linear death process, he applied the ideas to study diffusion. We extend the work of these authors by deriving expressions for the MAT for a general one-dimensional linear advection-diffusion-reaction problem. Using a combination of continuum and discrete approaches, we show that MAT and MPLT are equivalent for certain uniform-to-uniform transitions; these results provide a practical interpretation for MAT by directly linking the stochastic microscopic processes to a meaningful macroscopic time scale. We find that for more general transitions, the equivalence between MAT and MPLT does not hold. Unlike other critical time definitions, we show that it is possible to evaluate the MAT without solving the underlying partial differential equation (pde). This makes MAT a simple and attractive quantity for practical situations. Finally, our work explores the accuracy of certain approximations derived using MAT, showing that useful approximations for nonlinear kinetic processes can be obtained, again without treating the governing pde directly.

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## I. INTRODUCTION

Estimating a finite measure of the time taken for a particular advection-diffusion-reaction process to reach equilibrium is fundamental to many applications in the physical sciences. Such a time scale is called the critical time.

Here we briefly outline two practical examples for which the concept of critical time is very useful. First we consider the motion of fluid within a porous medium, which is governed by advection-diffusion partial differential equations (pdes) [1]. An important question currently faced by coastal water resource managers is to estimate the time required for the distribution of fresh and saline fluids in a coastal aquifer to respond to sea-level rise [2,3]. Second, we consider the formation of tissues and organs in a developing organism. These processes depend on the spatiotemporal regulation of cell behavior that is, in turn, thought to be regulated by gradients of chemical signaling molecules called morphogens [4]. These morphogen gradients are controlled by reaction-diffusion mechanisms [4,5], and one of the key questions is to determine whether the spatial distribution of morphogens reach steady state on time scales that are relevant for developmental patterning [6]. As these seemingly disparate examples indicate, estimating critical time scales for advection-diffusion-reaction equations has broad significance to any physical process that is governed by an advection-diffusion-reaction mechanism. Instead of focusing on any one particular example, here we investigate critical times for a range of linear and nonlinear advection-diffusion-reaction processes, presenting our analysis in a general framework to emphasize the broad applications of our results.

The concept of local accumulation time (LAT) was introduced by Berezhkovskii and co-workers [7–10]. Berezhkovskii considered a one–dimensional reaction-diffusion pde that was motivated by studying morphogen gradient formation [7–10]. Berezhkovskii solved the pde to give the time-dependent solution, $C(x,t)$, and the steady-state solution, $C_\infty(x) = \lim_{t\to\infty} C(x,t)$. A mathematical expression for the LAT, $\tau(x)$, was obtained, and Berezhkovskii argued that the LAT gives a measurement of time after which the transient solution becomes sufficiently close to the steady-state solution [8,9]. Therefore, the LAT is an estimate of the critical time for this problem.

Other definitions of critical time have been considered recently by Hickson and co-workers, who presented a thorough analysis of a one-dimensional linear reaction-diffusion pde on a finite domain [11–14]. Similar to the problem considered by Berezhkovskii, Hickson was able to solve the pde for both $C(x,t)$ and $C_\infty(x)$. With these solutions, Hickson sought to investigate a variety of measures of the time taken for the transient solution to approach the steady-state solution. Hickson used the term critical time, $t_c$, and considered three definitions for $t_c$: (1) the time taken for the averaged time-dependent profile to reach a particular proportion of the averaged steady-state solution; (2) the time taken for the total mass in the system to reach some predefined constant; and (3) the time taken for the density at a fixed position to reach a certain threshold.

Although Hickson's three criteria are based on physically reasonable principles, each criterion suffers from the limitation that there is always some subjectivity associated with implementing it. For example, definition (3) involves identifying the time at which the transient density at a fixed position reaches a certain threshold value. To use this definition, two choices have to be made: first, we must choose which particular position we are going to examine, and second, we must choose the value of the threshold density. If we know $C_\infty(x)$ in advance, then we might select $t_c$ to be the time taken for $C(x_1,t)$ to reach within 1% of $C_\infty(x_1)$. The difficulty with this definition is that the choice of a 1% threshold is arbitrary; we could easily change the threshold to 0.1%, or 0.01%, and the value of $t_c$ might be very sensitive to this choice [15,16]. These subjectivity issues are completely circumvented by using Berezhkovskii's definition of LAT since the concept of LAT does not require any choice of threshold criteria. We also note that to calculate critical time Hickson requires the exact solution for $C(x,t)$, which limits the practical value of these particular definitions of $t_c$. It would be more practical to calculate the critical time without the need to solve the underlying pde.

In this work we demonstrate that Berezhkovskii's definition of LAT, $\tau(x)$, is identical to the previously established concept of mean action time (MAT), $T(x)$, that was first introduced by McNabb in 1991 [15,16]. McNabb's original work was motivated by considering a diffusion equation in the context of a heat-transfer problem from the food refrigeration industry. In particular, McNabb considered the problem of constructing a finite measure of the time taken for the temperature of an isotropic heat conductor, initially at a uniform temperature $T_1$, to reach a new uniform temperature $T_2$ after the conductor has been immersed in an ambient temperature $T_2$ [15,16]. It is well known that for such diffusion problems it takes an infinitely long time for the temperature to reach $T_2$ uniformly throughout the conductor. McNabb introduced the concept of MAT to estimate the critical time for this problem. The major attraction of MAT is that it is possible to solve for the MAT without solving the underlying pde for the transient solution [15,16].

After McNabb's initial work, Landman and McGuinness [17] applied the definition of MAT to nonlinear diffusion processes in 2000. Landman and McGuinness used the Kirchhoff transformation to derive an expression for $T(x)$ [17]. Although Landman and McGuinness did not evaluate $T(x)$ in the case of nonlinear diffusion, they used their definition to motivate a new mathematical justification for the approximation of an intractable nonlinear diffusion equation with a related, but tractable, linear diffusion equation [17]. Based on this argument, Landman and McGuinness developed approximate analytical insight into a range of physical problems, including the filtration of flocculated suspensions and water transport in human eye lenses [17,18].

Unfortunately, after the concept of MAT was first introduced in 1991, and then extended in 2000, we are unaware of any further developments regarding MAT until very recently. Motivated by observations from cell biology experiments [19–21], our research group has been deriving approximate mean-field pde models associated with the collective motion of populations of different sized cells [22]. Our most recent work identified a family of nonlinear diffusion equations, each of which aims to approximate the same physical system [23]. By using the results of Landman and McGuinness [17], we were able to show that our family of seemingly unrelated nonlinear diffusion equations were, in fact, mathematically related through the concept of MAT.

Motivated by integrating and extending the work of Berezhkovskii [7–9] and McNabb [15,16], the present work meets five aims: (1) we show that Berezhkovskii's definition of LAT [7] is equivalent to McNabb's definition of MAT [15]; (2) we extend the work of McNabb by deriving expressions for the MAT for a general one-dimensional linear advection-diffusion-reaction problem; (3) we show that, for a general problem, it is possible to solve for an exact expression for the MAT without solving the underlying pde model; (4) in an attempt to provide a more comprehensive understanding of the physical meaning of MAT, we use a combination of continuum and discrete approaches to relate MAT to the mean particle lifetime (MPLT), and (5) based on observations associated with the linear advection-diffusion-reaction model, we give approximate equations governing the MAT for a nonlinear advection-diffusion-reaction model with a nonlinear decay term.

### A. Mean action time for linear diffusion processes and relationship to local accumulation time

To motivate our work we recall how MAT is defined for a linear diffusion process. For simplicity we work with a one-dimensional pde and note that all arguments can be extended to higher dimensions with isotropic transport coefficients [17]. We first consider a linear diffusion process governing the evolution of some density profile, $C(x,t)$. The diffusion equation can be written as

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}, \quad 0 < x < L, \tag{1}$$

where $D$ is the diffusivity. When we apply Eq. (1) to a situation with a particular initial condition, $C(x,0) = C_0(x)$, and boundary conditions such that the solution evolves toward some steady-state profile, $C_\infty(x) = \lim_{t\to\infty} C(x,t)$, we are interested to construct a finite measure of how long it takes for the difference between the transient solution and the steady-state solution to decay to zero [15,16]. We use the mean value theorem to relate the first moment of $\partial(C(x,t) - C_\infty(x))/\partial t$ with a mean value $T(x)$. In this context we write

$$T(x)\int_0^\infty \frac{\partial[C(x,t) - C_\infty(x)]}{\partial t}\,\mathrm{d}t = \int_0^\infty t\frac{\partial[C(x,t) - C_\infty(x)]}{\partial t}\,\mathrm{d}t, \tag{2}$$

where $T(x)$ is the MAT. To solve for $T(x)$ we use integration by parts on the right-hand side of Eq. (2) and, assuming that $C(x,t) - C_\infty(x) = o(t^{-1})$ as $t \to \infty$, we obtain

$$T(x) = \frac{1}{C_\infty(x) - C_0(x)}\int_0^\infty C_\infty(x) - C(x,t)\,\mathrm{d}t, \tag{3}$$

for $C_\infty(x) \neq C_0(x)$. Equation (3) is a general expression for the MAT that is independent of the initial condition, the boundary conditions, and the details of the governing equation. At this stage it is straightforward to note that Berezhkovskii's definition of LAT,

$$\tau(x) = \int_0^\infty \frac{C(x,t) - C_\infty(x)}{C_0(x) - C_\infty(x)} \, dt, \tag{4}$$

is identical to Eq. (3). We note that Berezhkovskii's work [8–10] considered a specific application of a reaction-diffusion equation where the initial condition was always $C_0(x) = 0$, and therefore that previous work always dealt with a more specific expression for $\tau(x)$.

Although it is possible to use Eq. (3) together with the solutions $C(x,t)$ and $C_\infty(x)$ to evaluate $T(x)$ [8,9], here we will show that we can solve for $T(x)$ directly without solving the underlying pde model. For example, we consider McNabb's original problem of placing an isotropic heat conductor, initially at uniform temperature $T_1$, in an environment with a different ambient temperature $T_2$. In the absence of any phase change the corresponding pde model for this process is Eq. (1) with a spatially constant initial condition and a spatially constant steady-state profile, so that $C_0(x) = C_0$ and $C_\infty(x) = C_\infty$. Under these conditions, we differentiate Eq. (3) twice with respect to $x$ and combine the resulting expression with Eq. (1) to obtain

$$T''(x) = -\frac{1}{D}, \tag{5}$$

where we have used prime notation to indicate differentiation with respect to $x$. The appropriate boundary conditions for Eq. (5) are $T(0) = T(L) = 0$, and the solution is

$$T(x) = \frac{x(L-x)}{2D}. \tag{6}$$

This solution for $T(x)$, shown in Fig. 1(b), provides us with a simple, convenient, and finite measure of the time taken for the initial disturbance to propagate through the system. We note that the arguments leading to this expression are very general and apply for all one-dimensional linear diffusion problems involving a transition from a spatially uniform initial condition to a spatially uniform steady state. We will call these kinds of transitions uniform-to-uniform transitions. The shape of the $T(x)$ profile is intuitive since we see that $T(x)$ is symmetric about the center of the domain, and $T(x)$ increases with distance away from either boundary. This agrees with our intuitive notion that a disturbance introduced simultaneously at $x = 0$ and $x = L$ would have an immediate effect at the boundaries, giving $T(0) = T(L) = 0$. Furthermore, we expect that the observation point that would take the longest time to be affected by this disturbance would be the center of the domain, where $x = L/2$. Finally, we see that $T(x)$ decreases with $D$, which is also intuitive since the rate at which information propagates through the system is proportional to $D$.

We will now extend these results for the linear diffusion model. In Sec. II we derive expressions for the MAT for a more general linear advection-diffusion-reaction pde model. In Sec. III we introduce a discrete stochastic random walk model that is related to the advection-diffusion-reaction equation analyzed in Sec. II, and we use this discrete model to investigate a relationship between the MAT and MPLT. In Sec. IV we investigate a practical application using the MAT by exploring an approximation introduced by Berezhkovskii [7] allowing us to approximate the long-term behavior of a pde solution with a simple exponential decay function related to $T(x)$. Based on the results in Sec. IV, we show that it is possible to formulate an approximate boundary value problem for the MAT associated with a nonlinear advection-diffusion-reaction problem in Sec. V. We compare a numerical approximation for $T(x)$ with the exact solution of our approximate model for the nonlinear advection-diffusion-reaction problem which indicates that the approximation gives a useful estimate of the MAT.

## II. MEAN ACTION TIME FOR LINEAR ADVECTION-DIFFUSION-REACTION PROCESSES

The original work by McNabb [15,16] and then Landman and McGuinness [17] considered the MAT for diffusion problems only; they did not consider MAT for more general problems involving transport by advection-diffusion or source terms in the pde model. Here we extend these previous investigations by considering a more general linear advection-diffusion-reaction problem given by

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - kC, \quad 0 < x < L, \tag{7}$$

where $D > 0$ is the diffusivity, $V$ is the advection velocity, and $k \geqslant 0$ is the reaction (death) rate. The general expression for the MAT, Eq. (3), still holds for the advection-diffusion-reaction problem. If we introduce $f(x) = C_\infty(x) - C_0(x)$, differentiate Eq. (3) twice with respect to $x$, and combine the resulting expression with Eq. (7), we obtain

$$T''(x) + \left(\frac{2f'(x)}{f(x)} - \frac{V}{D}\right)T'(x) + \left(\frac{f''(x)}{f(x)} - \frac{f'(x)V}{f(x)D} - \frac{k}{D}\right)T(x) = -\frac{1}{D}. \tag{8}$$

To solve Eq. (8) we introduce the transformation $S(x) = f(x)T(x)$, converting Eq. (8) into

$$S''(x) - \frac{V}{D}S'(x) - \frac{k}{D}S(x) = -\frac{f(x)}{D}, \tag{9}$$

which has constant coefficients and can be solved using standard techniques. We note that Eq. (9) describes the MAT for any one-dimensional linear advection-diffusion-reaction equation for a general transition from $C_0(x)$ to $C_\infty(x)$. Since many physical processes are governed by the linear advection-diffusion-reaction equation, the solution of Eq. (9) will be relevant to any discipline in the physical sciences where the linear advection-diffusion-reaction equation plays a role.

For a uniform-to-uniform transition we have constant $C_\infty(x) = C_\infty$, $C_0(x) = C_0$, and $f'(x) = f''(x) = 0$. Under these conditions the appropriate boundary conditions for Eq. (8) are $T(0) = T(L) = 0$, and the solution is

$$T(x) = Ae^{m^+x} + Be^{m^-x} + \frac{1}{k} \tag{10}$$

for $k > 0$, where

$$m^\pm = \frac{V}{2D} \pm \sqrt{\left(\frac{V}{2D}\right)^2 + \frac{k}{D}}, \quad A = \frac{e^{m^-L} - 1}{k(e^{m^+L} - e^{m^-L})}, \quad B = \frac{1 - e^{m^+L}}{k(e^{m^+L} - e^{m^-L})}. \tag{11}$$

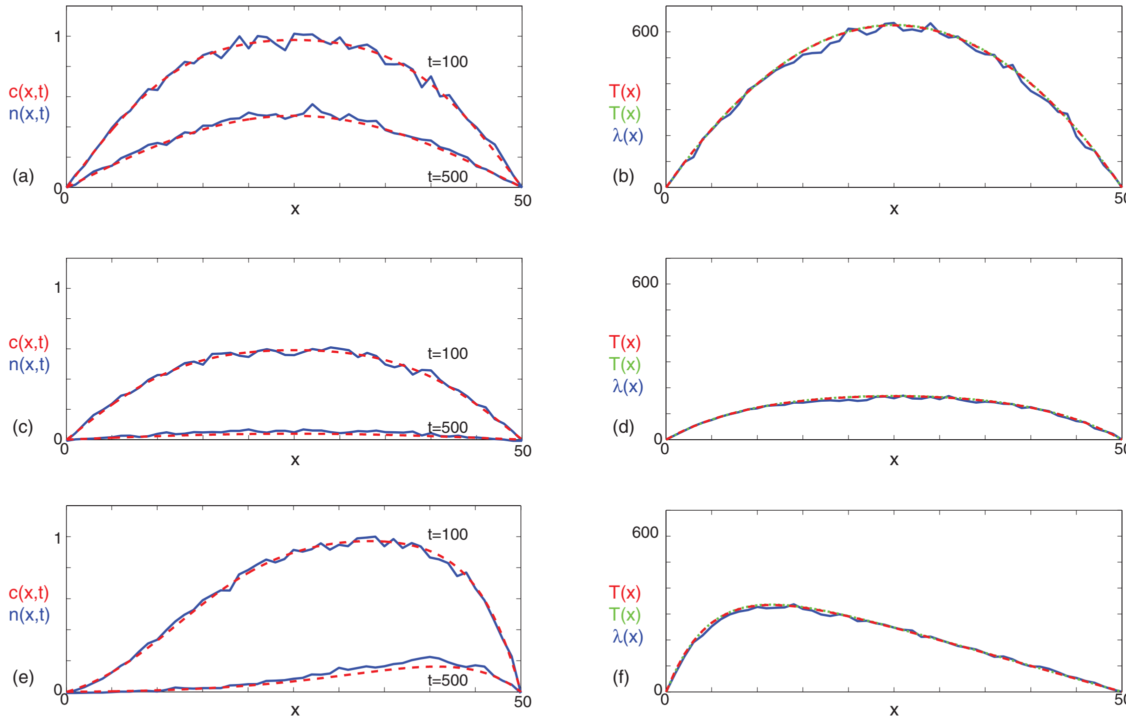


FIG. 1. (Color online) MAT for linear transport associated with a uniform-to-uniform transition on the finite domain $0 \leqslant x \leqslant 50$. Results in (a, b) correspond to the diffusion-only process ($D = 0.5, V = 0, k = 0$), results in (c, d) correspond to the diffusion-death process ($D = 0.5, V = 0, k = 0.005$), and results in (e, f) correspond to the diffusion-advection process ($D = 0.5, V = 0.1, k = 0$). For all problems we consider an initial condition $C_0(x) = 1$, and we apply homogeneous Dirichlet boundary conditions $C(0,t) = 0$ and $C(50,t) = 0$, giving $C_\infty(x) = 0$. Numerical solutions of Eq. (7), denoted $C(x,t)$, are given in red (dashed) in (a), (c), and (e) at $t = 100$ and $t = 500$, as indicated. Discrete density profiles from the stochastic random walk model, $n(x,t)$, are superimposed in (a), (c), and (e) at $t = 100$ and $t = 500$ are shown in blue (solid). Results in (b), (d), and (f) show the exact solution for $T(x)$ in red (dashed), a numerical approximation of Eq. (2) in green (dotted), and the MPLT calculated using the stochastic random walk algorithm is shown in blue (solid). All numerical results are obtained using the same technique outlined in the main text with $\delta x = 0.05$ and $\delta t = 0.1$. The stochastic random walk algorithm was implemented on a one-dimensional lattice with $\Delta = 1$, and the discrete results in (a, b) correspond to diffusion-only processes ($\epsilon = 0, d = 0$), results in (c, d) correspond to diffusion-reaction processes ($\epsilon = 0, d = 0.005$), and results in (e, f) correspond to diffusion-advection processes ($\epsilon = 0.05, d = 0$). All discrete simulations were initiated with 1000 particles located at each lattice site.

For the uniform-to-uniform transition with $k = 0$ and $T(0) = T(L) = 0$, the solution of Eq. (8) can be written as

$$T(x) = A + B\mathrm{e}^{\frac{Vx}{D}} + \frac{x}{V}, \tag{12}$$

where

$$A = \frac{L}{V\left(\mathrm{e}^{\frac{VL}{D}} - 1\right)}, \quad B = \frac{-L}{V\left(\mathrm{e}^{\frac{VL}{D}} - 1\right)}. \tag{13}$$

For the uniform-to-uniform transition with $k = 0$, $V = 0$ and $T(0) = T(L) = 0$, the solution of Eq. (8) is given by Eq. (6).

Equations (10) and (12) explicitly show how the processes of advection, diffusion, and reaction interact to give a more complex spatial distribution of $T(x)$ compared to the simple form we obtained previously for diffusion only [Eq. (6)].

To visualize the MAT for advection-diffusion-reaction problems, we plot various numerical solutions of Eq. (7) in Figs. 1(a), 1(c), and 1(e). These three solutions correspond to diffusion-only, advection-diffusion, and diffusion-reaction processes, respectively. In each case we consider a spatially uniform initial condition, $C(x,0) = 1$, on a finite domain, $0 \leqslant x \leqslant 50$. Homogeneous Dirichlet boundary conditions are applied so that we have $C(0,t) = 0$, $C(50,t) = 0$, and $C_\infty(x) = 0$. Numerical solutions of Eq. (7) are obtained using a finite difference approximation, with central differences, on a uniformly discretized domain with grid size $\delta x$ [24]. A backward Euler method is used to march the numerical solution forward in time with time increment $\delta t$. The solutions of Eq. (7), shown in Figs. 1(a), 1(c), and 1(e), clearly reflect the differences in the processes in each case. In Fig. 1(a), with diffusion only, we see that the transient solution is symmetric about the center of the domain. In Fig. 1(c) with diffusion and death, we see that the solution is also symmetric about the center of the domain, except now the solution evolves toward the steady state faster than the diffusion-only results in Fig. 1(a); this difference is caused by the death term in Eq. (7). The profiles in Fig. 1(e) clearly demonstrate the effect of advective transport, since the profiles are asymmetric about the center of the domain. This asymmetry is caused by the advection flux, which acts to transport the density profile in the positive $x$ direction.

In addition to the numerical solutions of Eq. (7), we plot the corresponding $T(x)$ profile in Figs. 1(b), 1(d), and 1(f). Figure 1(b) shows the $T(x)$ profile given by Eq. (6) which we have discussed previously in Sec. I A. Figure 1(d) shows the corresponding $T(x)$ profile for the diffusion-death results given by Eq. (10). We see that $T(x)$ is symmetric about the center of the domain and that for each fixed value of $x$ the MAT is smaller for the diffusion-death case compared to the diffusion-only case in Fig. 1(b). This is intuitively reasonable, since we know that the death term in Eq. (7) acts to increase the rate at which the initial condition evolves toward the steady-state profile, as we saw in the numerical profiles given in Figs. 1(a) and 1(c). Figure 1(f) shows the MAT profile for advection-diffusion transport given by Eq. (12), and here we see that the MAT profile is asymmetric about the center of the domain. This solution implies that regions near the left-hand boundary take a longer time to evolve toward the steady-state solution profile than regions near the right-hand boundary.

## III. INTERPRETATION OF MEAN ACTION TIME

In his original work, McNabb [15,16] motivated the idea of MAT by first considering an ordinary differential equation (ode) model of a linear death process,

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -kC, \tag{14}$$

where $k > 0$ is the death rate. McNabb introduced the idea of MAT by noting that the solution of Eq. (14), $C(t) = C(0)\mathrm{e}^{-kt}$, takes an infinite amount of time to reach the theoretical steady-state value and he showed that, according to Eq. (2), the MAT for Eq. (14) is simply $T = 1/k$. McNabb commented that $1/k$ corresponds to the MPLT for this linear death process. Here we aim to explore the relationship between MPLT and MAT for spatially variable processes governed by a pde model rather than a spatially invariant ode model.

### A. Discrete random walk approach to evaluate the mean particle lifetime

To explore the relationship between MAT and MPLT, we introduce a stochastic random walk that is related to Eq. (7) and aim to reproduce the continuum pde results in Fig. 1 using the stochastic approach. To do this we consider a one-dimensional lattice with lattice spacing $\Delta$. Each lattice site is indexed $i$, where $i \in \mathbb{Z}^+$, so that the position of each lattice site is $x = i\Delta$. Agents can die, and do so with probability per unit time $d \in [0,1]$. Agents hop in the positive or negative $x$ directions with probability per unit time $(1/2 \pm \epsilon)$.

To simulate the process we use a Gillespie algorithm [25]. We simulate the uniform-to-uniform transition problem in Fig. 1 by setting $\Delta = 1$ so that we have a lattice with 51 sites. Each site is initially occupied with $n_{\max}$ particles. As the Gillespie algorithm proceeds, we remove any agent that resides in the first ($i = 1$) and final ($i = 51$) lattice sites so that the discrete algorithm mimics the effects of the homogeneous Dirichlet boundary conditions imposed in Fig. 1. To extract the approximate density profiles from the discrete algorithm, we record the number of particles at the $i$th lattice site and normalize with $n_{\max}$ to give

$$n(x,t) = \frac{\hat{n}(x,t)}{n_{\max}}, \tag{15}$$

where $\hat{n}(x,t)$ is the number of particles at the lattice site at position $x$ at time $t$.

Using standard arguments to relate the random walk model to a pde description of the process [26–28], we expect that the distribution of agents in the system will, on average, be related to Eq. (7), where

$$D = \lim_{\Delta\to 0} \frac{\Delta^2}{2}, \quad V = \lim_{\Delta\to 0} 2\Delta\epsilon, \quad k = \lim_{\Delta\to 0} d. \tag{16}$$

To obtain a well-defined continuum limit, we must have the motility bias and death rate decrease to zero as $\epsilon = \mathcal{O}(\Delta)$ and $d = \mathcal{O}(\Delta^2)$ [27–29]. On our lattice with $\Delta = 1$, we have $D = 1/2$, $V = 2\epsilon$, and $k = d$, and our results in Figs. 1(a), 1(c), and 1(e) show that the solution of Eq. (7) matches the discrete profiles of $n(x,t)$ very well.

In addition to estimating the agent density profiles, we also calculate the MPLT with the discrete random walk algorithm by recording, for each lattice site $i$, the time taken for every particle that originated at that particular site to leave the system, either by moving out of one of the Dirichlet boundaries or through a death event. To characterize the MPLT we consider initiating a simulation with $n_{\max}$ particles in each lattice site; we then record the particle lifetime for all $n_{\max}$ particles for each lattice site. Averaging the particle lifetimes gives an estimate of the MPLT:

$$\lambda(x) = \frac{1}{n_{\max}} \sum_{j=1}^{n_{\max}} t_j(x), \tag{17}$$

where $t_j(x)$ is the time taken for the $j$th particle that was originally placed at position $x$ to leave the system. Results in Figs. 1(b), 1(d), and 1(f) compare the MAT and MPLT for diffusion-only, diffusion-death, and advection-diffusion processes, respectively. In all cases we see that there is a very good correspondence between the continuum MAT profile and the discrete MPLT profile, and this indicates that the MAT and MPLT for these processes are identical. This observation is consistent with McNabb's conjecture about the equivalence of MAT and MPLT for the linear death ode model [Eq. (14)]. Motivated by the comparison of MAT and MPLT in Fig. 1, we will derive a mathematical expression for MPLT in Sec. III B.

### B. Analytical estimate of the mean particle lifetime

Following [29,30], we now outline an argument that leads to a boundary value problem describing the MPLT for a one-dimensional biased random walk with death. We consider a one-dimensional biased random walk on $\{0,\Delta,2\Delta,\ldots,N\Delta\}$, and suppose that we have absorbing boundaries at $x = 0$ and $x = N\Delta$. For this process, agents move left with probability per unit time $P_l$, agents move right with probability per unit time $P_r$, agents die with probability per unit time $P_d$, such that $P_l + P_r + P_d = 1$. To estimate the MPLT, we develop an expression describing the mean number of steps taken before the particle leaves the domain.

Let $\mathbb{E}(i)$ be the average number of steps taken before being absorbed at either boundary or dying, given that the random walker starts at site $i$. We derive an expression for $\mathbb{E}(i)$ by conditioning on the first event being a jump in either direction or a death event:

$$\begin{aligned}\mathbb{E}(i) &= \mathbb{E}(i|\text{first event is a jump to the left})P_l \\ &\quad + \mathbb{E}(i|\text{first event is a jump to the right})P_r \\ &\quad + \mathbb{E}(i|\text{first event is death})P_d \\ &= [1+\mathbb{E}(i+1)]P_l + [1+\mathbb{E}(i-1)]P_r + [1+\mathbb{E}(0)]P_d,\end{aligned} \tag{18}$$

where we have used the boundary conditions $\mathbb{E}(0) = 0$ and $\mathbb{E}(N) = 0$ to give the final term in Eq. (18). We will now convert this discrete statement into a continuum equation by identifying the discrete lifetime, $\mathbb{E}(i)$, with the continuous description $E(x)$. Expanding in a truncated Taylor series,

$$E(x \pm \Delta) = E(x) \pm \Delta E'(x) + \frac{\Delta^2}{2}E''(x) + \mathcal{O}(\Delta^3), \tag{19}$$

we combine Eqs. (18) and (19) to obtain

$$\begin{aligned}-1 &= \frac{\Delta^2}{2}(P_l + P_r)E''(x) + \Delta(P_l - P_r)E'(x) \\ &\quad + (P_l + P_r - 1)E(x).\end{aligned} \tag{20}$$

Recalling that $P_l + P_r + P_d = 1$, we can rewrite Eq. (20) as

$$E''(x) - \frac{V}{D}E'(x) - \frac{k}{D}E(x) = -\frac{1}{D}, \tag{21}$$

where

$$\begin{aligned}&D = \lim_{\Delta\to 0}\frac{\Delta^2}{2}(P_l + P_r), \quad V = \lim_{\Delta\to 0}\Delta(P_r - P_l), \\ &k = \lim_{\Delta\to 0}P_d.\end{aligned} \tag{22}$$

For all our discrete simulations in Fig. 1 we had $\Delta = 1$, $P_l + P_r = 1$, and $P_r - P_l = 2\epsilon$ so that $D = 1/2$ and $V = 2\epsilon$ in Eq. (21). Under these conditions the equation governing the MPLT [Eq. (21)] is identical to the equation governing the MAT for a uniform-to-uniform transition [Eq. (8) with $f'(x) = f''(x) = 0$]. The correspondence between the governing equations for MPLT and MAT explains why the computational estimates of MPLT in Figs. 1(b), 1(d), and 1(f) compared very well with the exact solution for the MAT. These arguments also lead us to anticipate that the MAT and MPLT for a nonuniform transition will not be equivalent. For nonuniform transitions we have $f'(x) \neq 0$ and $f''(x) \neq 0$, which means that Eq. (8) is different from Eq. (21), and so we expect that MAT and MPLT will no longer be equivalent for these more general transitions.

### C. Nonuniform transitions

All results presented in Fig. 1, as well as all previous results considered by McNabb [15,16] and Landman and McGuinness [17], correspond to a uniform-to-uniform transition. We note that Berezhkovskii and co-workers were interested in a uniform-to-nonuniform transition, and here we extend the application of MAT to more general problems that will provide further insight into our physical interpretation of MAT.

#### *1. Nonuniform-to-uniform transition*

We first consider the same geometry and boundary conditions used for the problems in Fig. 1, except now we impose a different initial condition, $C_0(x) = x/L$, which leads to the trivial steady-state solution $C_\infty(x) = 0$. To demonstrate the key effects of the nonuniform-to-uniform transition, we will consider linear diffusion [$V = k = 0$ in Eq. (7)] and note that our analysis can be extended to consider advective transport or the linear death term if necessary. Under these conditions, Eq. (8) simplifies to

$$T''(x) + \frac{2T'(x)}{x} = -\frac{1}{D}. \tag{23}$$

At $x = L$, our choice of boundary conditions and initial conditions in the pde means that we must have $T(L) = 0$. Given that we expect $T(x)$ to remain finite on the entire domain, Eq. (23) implies the other condition must be $T'(0) = 0$, and thus the solution is

$$T(x) = \frac{L^2 - x^2}{6D}. \tag{24}$$

We note that, unlike the uniform-to-uniform diffusion-only problem [Eq. (6)], $T(x)$ for the nonuniform-to-uniform transition is asymmetric about the center of the domain.

We present a suite of continuum and discrete results for the nonuniform-to-uniform transition problem in Figs. 2(a) and 2(b). In Fig. 2(a) we solve the linear diffusion equation [Eq. (7) with $V = k = 0$] on $0 \leqslant x \leqslant 50$ with $C(x,0) = x/50$, $C(0,t) = 0$, and $C(50,t) = 0$. Equivalent results from the discrete random walk algorithm are superimposed, and we observe an excellent match between the continuum density solutions and the discrete random walk results. In Fig. 2(b) we present the exact solution for the MAT [Eq. (24)] as well as the MPLT solution from the random walk algorithm. Unlike the results in Fig. 1, here we see that the MAT is not equivalent to the MPLT for this problem.

To provide an additional check on Eq. (24), we generate a numerical approximation of MAT directly from Eq. (2) by numerically approximating the improper integrals. We use our finite difference code that generates the numerical solution of Eq. (7). To do this we approximate Eq. (2) with a similar expression by using

$$\begin{aligned}T(x)\int_0^{t_l}\frac{\partial[C(x,t) - C_\infty(x)]}{\partial t}\,dt \\ = \int_0^{t_l} t\,\frac{\partial[C(x,t) - C_\infty(x)]}{\partial t}\,dt,\end{aligned} \tag{25}$$

where we have replaced the upper integration limit with a large, but finite, value $t_l$. We then approximate the proper integrals in Eq. (25) using the trapezoid rule. We computed $T(x)$ using Eq. (25) with a careful choice of $t_l = 10\,000$. We chose this particular value of $t_l$ by performing a number of numerical computations where we systematically increased the value of $t_l$ until we observed that the $T(x)$ profile converged as $t_l$ was chosen to be sufficiently large. A numerical approximation of $T(x)$ is included in Fig. 2(b), and we see that it is identical to the profile given by Eq. (24).

We remark that the difference between the MPLT and MAT in Fig. 2(b) had been anticipated previously, since the equation governing the MPLT [Eq. (21)] does not depend on the initial configuration of the agents on the lattice whereas the equation governing the MAT [Eq. (8)] depends on the initial condition $C_0(x)$. This difference explains why the

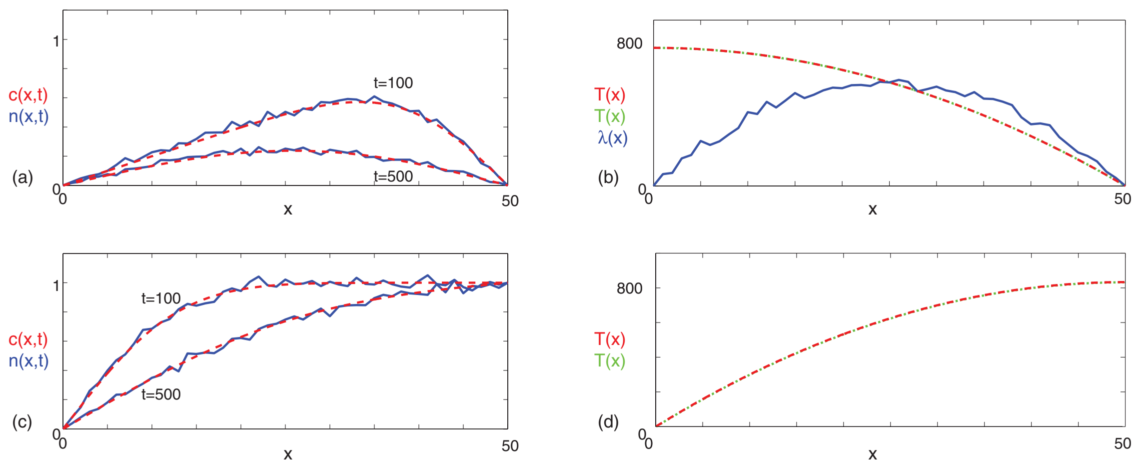


FIG. 2. (Color online) MAT for linear diffusion associated with a nonuniform-to-uniform transition in (a, b) and a uniform-to-nonuniform transition in (c, d). All results are on the finite domain $0 \leqslant x \leqslant 50$. Results in (a) correspond to diffusion-only ($D = 0.5, V = 0, k = 0$) with $C_0(x) = x/50$, $C(0,t) = 0$, $C(50,t) = 0$, and $C_\infty(x) = 0$. Numerical solutions of Eq. (7) are given in red (dashed) and are superimposed on the corresponding discrete profile, $n(x,t)$, shown in blue (solid). Results in (b) show the exact solution for $T(x)$ in red (dashed), a numerical approximation of Eq. (2) in green (dotted), and the MPLT in blue (solid) that was calculated using the stochastic random walk algorithm. Results in (c) correspond to diffusion-only ($D = 0.5, V = 0, k = 0$) with $C_0(x) = 1$, $C(0,t) = 0$, $C(50,t) = 1$, and $C_\infty(x) = x/50$. Numerical solutions of Eq. (7) are given in red (dashed) and are superimposed on the corresponding discrete profile, $n(x,t)$, shown in blue (solid). Results in (d) show the exact solution for $T(x)$ in red (dashed) and a numerical approximation of Eq. (2) in green (dotted). All numerical results are obtained using the same technique outlined in the main text with $\delta x = 0.025$ and variable $\delta t$, with $1 \times 10^{-5} \leqslant \delta t \leqslant 1$. The stochastic random walk algorithm was implemented on a one-dimensional lattice with $\Delta = 1$. All discrete results correspond to ($\epsilon = 0, d = 0$), discrete simulations in (a, b) were initiated by placing $200i$ particles at the $i$th lattice site, whereas the discrete results in (c, d) were initiated by placing 1000 particles at each lattice site.

exact solution for the MAT does not compare well with the computational estimate of MPLT in Fig. 2. In fact, we see that the computational estimates of the MPLT for the nonuniform-to-uniform transition in Fig. 2(b) appears to be equivalent to the computational estimates of the MPLT for the uniform-to-uniform transition in Fig. 1(b). This is consistent with Eq. (21), which shows that the MPLT is independent of the initial distribution of agents on the lattice. We note that our continuum-discrete comparisons in Figs. 1 and 2 were motivated by McNabb's conjecture that MAT and MPLT were identical for a linear decay ode model. A very recent study presented a similar discrete approach to interpret LAT in terms of first passage times [10,31] but did not consider the relationship between MPLT and MAT.

In summary, the results in Fig. 2(b) indicate that MAT and MPLT for the nonuniform-to-uniform problem are not equivalent. This observation is of interest, since McNabb's original work was motivated by noting that the MAT for the linear death ode [Eq. (14)] was equivalent to the MPLT. Our results in Fig. 1 for the uniform-to-uniform transition problem corroborate McNabb's observations; however, our results for the nonuniform-to-uniform problem in Fig. 2(b) indicate that the MAT and MPLT are not always equivalent.

#### 2. *Uniform-to-nonuniform transition*

To compliment the results in Sect. III C1, we now consider the same initial condition used in Fig. 1, except we impose different boundary conditions, given by $C(0,t) = 0$ and $C(L,t) = 1$. Considering diffusion [$V = k = 0$ in Eq. (7)], we obtain a nonuniform steady state, $C_\infty(x) = x/L$. For these conditions, Eq. (8) simplifies to

$$T''(x) + \frac{2T'(x)}{(x - L)} = -\frac{1}{D}. \tag{26}$$

At $x = 0$, our choice of boundary conditions and initial conditions in the pde means that we must have $T(0) = 0$, while the condition that $T(x)$ remains finite gives $T'(L) = 0$. Thus, the solution of Eq. (26) is

$$T(x) = \frac{x(2L - x)}{6D}. \tag{27}$$

As before, we see that $T(x)$ for the uniform-to-nonuniform transition is asymmetric about the center of the domain. We present a suite of continuum and discrete results for the uniform-to-nonuniform transition problem in Figs. 2(c) and 2(d). In Fig. 2(c) we solve the linear diffusion equation [Eq. (7) with $V = k = 0$] with $C(x,0) = 1$ on $0 \leqslant x \leqslant 50$ with $C(0,t) = 0$ and $C(50,t) = 1$. Equivalent results from the discrete random walk algorithm are superimposed and show that we have an excellent match between the continuum density solutions and the discrete random walk results. In Fig. 2(d) we present the exact solution for the MAT [Eq. (27)] as well as the numerical approximation of $T(x)$ evaluated using Eq. (25). The two profiles in Fig. 2(d) are indistinguishable, which confirms that Eq. (27) accurately predicts the MAT for this problem.

We did not use the random walk algorithm to compute the MPLT for the uniform-to-nonuniform problem. For all previous cases considered in this work, we always had the same trivial steady-state solution, $C_\infty(x) = 0$. Under these conditions, we expect that if we run the corresponding discrete algorithm for a sufficiently long period of time, then eventually all agents will have left the system so that it is straightforward to compute the particle lifetime using Eq. (17). For the uniform-to-nonuniform transition problem, we have $C_\infty(x) = x/L$, which means that as the discrete algorithm proceeds, there is always a finite number of agents remaining in the system for all time and we cannot evaluate the MPLT with Eq. (17) like we did in the simpler cases for which $C_\infty(x) = 0$.

#### 3. More general transitions

Results in Figs. 1 and 2 correspond to relatively straightforward transitions for which $C_0(x)$ and $C_\infty(x)$ are either constant or linear functions of $x$. Here we provide further results for a more detailed problem with a different steady-state profile. To do this we consider Eq. (7) with $V = 0$ on $0 \leqslant x \leqslant L$, with $\partial C/\partial x = 0$ at $x = 0$ and $C(L,t) = 1$. This particular problem is frequently encountered in the chemical engineering literature as a model of a chemical reaction in a porous catalyst [32–34]. The steady-state solution is given by

$$C_\infty(x) = \frac{\cosh\left(x\sqrt{k/D}\right)}{\cosh\left(L\sqrt{k/D}\right)}. \tag{28}$$

We now evaluate the MAT for two initial conditions: (1) $C_0(x) = 0$ and (2) $C_0(x) = 1$. With appropriate boundary conditions, $T'(0) = 0$ and $T(L) = 0$, the MAT for the transition from $C_0(x) = 0$ to Eq. (28) is given by

$$T(x) = \frac{x}{D\sqrt{k/D}(1+\exp[2x\sqrt{k/D}])} - \frac{x}{2D\sqrt{k/D}} + \frac{L(\exp[2L\sqrt{k/D}]-1)}{D\sqrt{k/D}(\exp[2x\sqrt{k/D}]+1)}. \tag{29}$$

With an appropriate Robin boundary condition, $-2\sqrt{D/k}\tanh(L\sqrt{k/D})T'(L) = T(L)$, the MAT for the transition from $C_0(x) = 1$ to Eq. (28) is given by

$$T(x) = \frac{L\sinh(L\sqrt{k/D})\cosh(x\sqrt{k/D}) - x\sinh(x\sqrt{k/D})\cosh(L\sqrt{k/D})}{2D\sqrt{k/D}\cosh(L\sqrt{k/D})[\cosh(x\sqrt{k/D}) - \cosh(L\sqrt{k/D})]} + \frac{1}{k}. \tag{30}$$

Results for $C_0(x) = 0$ [Figs. 3(a) and 3(b)] show a transient evolution, $C(x,t)$, that accumulates toward the steady-state profile. This behavior is very similar to the examples studied by Berezhkovskii and co-workers [7–9], which led them to call their definition $\tau(x)$ the local accumulation time, since it gives a measure of the amount of time that it takes the transient profile to accumulate toward the steady-state solution. Conversely, results for $C_0(x) = 1$ [Figs. 3(c) and 3(d)] involve a transient solution, $C(x,t)$, that decays toward the steady-state profile. This behavior is qualitatively the opposite of the accumulation-type behavior studied by Berezhkovskii and co-workers [7–9]. Despite these differences, our results show that the relevant solutions of Eq. (8) and the numerical evaluation of $T(x)$, using Eq. (25) with $t_l = 10\,000$, are equivalent. These additional results illustrate the generality of MAT, showing that it can be applied to more detailed transitions that are associated with both accumulation-like and decay-like transient behavior.

## IV. PRACTICAL APPLICATION OF MEAN ACTION TIME

In addition to proposing the concept of LAT, Berezhkovskii introduced a relatively straightforward approximation whereby he used $T(x)$ to approximate the solution of the underlying pde model. Berezhkovskii [7] introduced the following equality:

$$T(x) = \int_0^\infty \frac{C(x,t) - C_\infty(x)}{C_0(x) - C_\infty(x)}\,\mathrm{d}t = \int_0^\infty \mathrm{e}^{-\frac{t}{T}}\,\mathrm{d}t. \tag{31}$$

Motivated by Eq. (31), Berezhkovskii assumed that the integrands in Eq. (31) are approximately equal. This gives

$$C(x,t) \approx C_\infty(x)(1 - \mathrm{e}^{-\frac{t}{T}}) + C_0(x)\mathrm{e}^{-\frac{t}{T}}. \tag{32}$$

We will examine the effectiveness of Berezhkovskii's approximation by revisiting the problems previously considered in Fig. 1. To provide additional insight into these problems, we solve Eq. (7) on $0 \leqslant x \leqslant L$, with $C(x,0) = 1$ and $C(0,t) = C(L,t) = 0$, using separation of variables and Fourier series and obtain

$$C(x,t) \sim \left[\frac{8\pi D^2\left(1+\mathrm{e}^{\frac{-VL}{2D}}\right)}{(VL)^2 + (2\pi D)^2}\right]\sin\left(\frac{x\pi}{L}\right) \times \mathrm{e}^{\frac{Vx}{2D}}\mathrm{e}^{-\frac{\pi^2 Dt}{L^2}}\mathrm{e}^{-\frac{V^2}{4D}t}\mathrm{e}^{-kt} \quad \text{as} \quad t \to \infty. \tag{33}$$

We call Eq. (33) the leading eigenvalue approximation [13], and we note that this approximation corresponds to retaining the first term in the series solution.

Results in Fig. 4 consider a suite of uniform-to-uniform transitions that correspond with those results presented in Fig. 1 for diffusion-only, diffusion-death, and advection-diffusion, respectively. In Fig. 4 we compare the numerical solutions for $C(x,t)$ with the two approximations given by Eqs. (32) and (33). Profiles are compared for two fixed values of $x$ ($x = 10$ and $x = 25$), and in each subfigure we show the corresponding value of $T(x)$ associated with that particular problem. In all cases we see that the numerical solution of the full problem can be approximated very accurately by the leading eigenvalue approximation for sufficiently large values of $t$, as expected. Similar to Berezhkovskii [7], we observe that the accuracy of the approximate exponential decay solution, given by Eq. (32), is problem dependent and parameter dependent. For example, with the diffusion-death results in Figs. 4(c) and 4(d) [Eq. (7) with $V = 0$], we see that Berezhkovskii's approximate exponential solution provides an excellent approximation to the full numerical solutions for all values of $t$ considered, whereas the diffusion-only

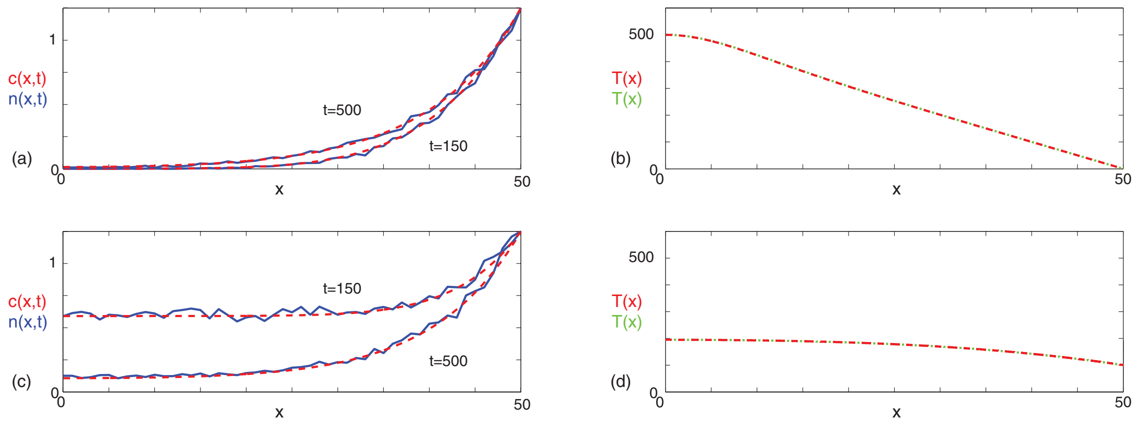


FIG. 3. (Color online) MAT for linear diffusion reaction ($D = 0.5, V = 0, k = 0.005$) on $0 \leqslant x \leqslant 50$, with $\partial C/\partial x = 0$ at $x = 0$ and $C(50,t) = 1$. The solution evolves to $C_\infty(x) = \cosh(x\sqrt{k/D})/\cosh(50\sqrt{k/D})$. Results in (a, b) correspond to $C_0(x) = 0$ (accumulation), and results in (c, d) correspond to $C_0(x) = 1$ (decay). Numerical solutions of Eq. (7), $C(x,t)$, are given in red (dashed) in (a) and (c) at $t = 150$ and $t = 500$, as indicated. Discrete density profiles from the stochastic random walk model, $n(x,t)$, are shown in blue (solid) in (a) and (c) at $t = 150$ and $t = 500$. Results in (b) and (d) show the exact solution for $T(x)$ in red (dashed) and a numerical approximation of Eq. (2) in green (dotted). All numerical results are obtained using the same technique outlined in the main text with $\delta x = 0.025$ and variable $\delta t$, with $1 \times 10^{-5} \leqslant \delta t \leqslant 1$. The stochastic random walk algorithm was implemented with $\epsilon = 0$ and $d = 0.005$ on a one-dimensional lattice with $\Delta = 1$. Discrete simulations in (a) were initiated with zero particles located at each lattice site, while discrete simulations in (c) were initiated with 1000 particles located at each lattice site.

results in Figs. 4(a) and 4(b) [Eq. (7) with $V = k = 0$] indicate that Berezhkovskii's exponential solution is a poor approximation to the true solution. It is difficult to draw specific conclusions about the usefulness of Berezhkovskii's approximation, since we know that the assumptions leading to Eq. (32) are approximate only.

We note in passing that, given the leading eigenvalue term in Eq. (33), we can approximate the MAT using Eq. (3) to give

$$T(x) \approx \left(\frac{\pi^2 D}{L^2} + \frac{V^2}{4D} + k\right)^{-1}\left[\frac{8\pi\left(1 + e^{\frac{-VL}{2D}}\right)}{(VL/D)^2 + (2\pi)^2}\right] \times \sin\left(\frac{x\pi}{L}\right)e^{\frac{Vx}{2D}}. \qquad (34)$$

In a similar fashion to the argument just given, Eq. (34) can provide a reasonable approximation for certain parameter values. Further, by defining the Péclet number as $\mathrm{Pe} = VL/D$, the simplified expression for MAT [Eq. (34)] neatly shows how MAT can be related to the three important time scales in the problem: namely, the diffusive time scale $t_D = (D/L^2)^{-1}$; the advective time scale $t_A = (V^2/D)^{-1}\mathrm{Pe}$; and the reaction time scale $t_R = k^{-1}$. This highlights that $t_D$ dominates (is smaller) when $t_A$ and $t_R$ are large. However, it is important to emphasize that the derivation of Eq. (34), and derivations of similar approximations for other critical times [11–13], requires prior knowledge of the full solution of the underlying pde model. On the other hand, the use of MAT has the significant benefit that we are able to compute the MAT without solving the underlying pde model.

## V. NONLINEAR DECAY

To extend the practical application of the concept of MAT, it is instructive to consider a more general problem with a nonlinear source term:

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - V\frac{\partial C}{\partial x} - kC^n, \quad 0 < x < L, \qquad (35)$$

where $n > 0$ is the order of the reaction. This kind of nonlinear advection-diffusion-reaction model is frequently encountered in many areas of physical sciences, including modeling chemical reaction processes in a catalyst [32–35], gas-solid reactions [36,37], and combustion [38]. This nonlinear decay term is also associated with surface reactions, such as adsorption [39,40] that are important in modeling bioremediation processes and contaminant transport in aquifers [41]. Studying Eq. (35) will allow us to show how the traditional definitions of MAT (and LAT) cannot, in general, be applied directly to nonlinear transport equations. Nonetheless, the insight we developed by considering linear problems will allow us to develop useful approximations of $T(x)$ for Eq. (35).

For a uniform-to-uniform transition, the boundary value problem for $T(x)$ can be written as

$$T''(x) + \frac{V}{D}T'(x) - \frac{k}{D}\int_0^\infty C^n(x,t)\,dt = -\frac{1}{D}. \qquad (36)$$

As it stands, we cannot solve Eq. (36) since the governing equation for $T(x)$ depends explicitly on $\int_0^\infty C(x,t)^n\,dt$. However, we know that Eq. (31) is exact, and thus proceed by making the assumption

$$\int_0^\infty C^n(x,t)\,dt \approx \int_0^\infty e^{-\frac{nt}{T}}\,dt = \frac{T(x)}{n}, \qquad (37)$$

which allows us to approximate Eq. (36) by

$$T''(x) + \frac{V}{D}T'(x) - \frac{k}{nD}T(x) = -\frac{1}{D}. \qquad (38)$$

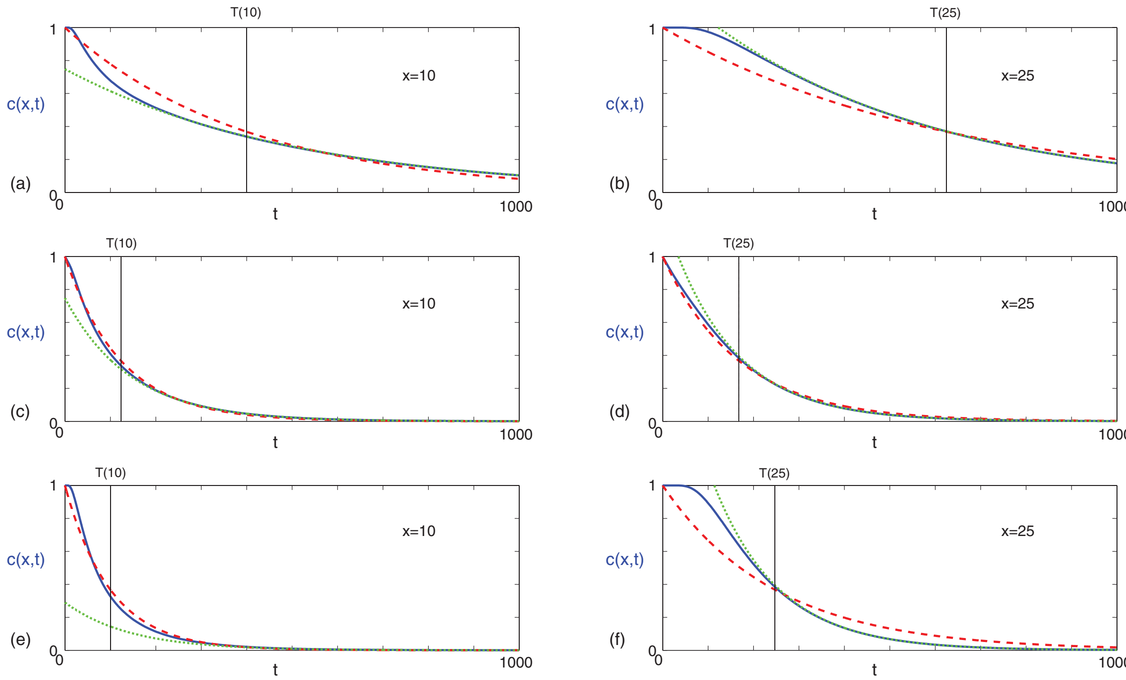


FIG. 4. (Color online) Profiles in (a, b), (c, d), and (e, f) compare a numerical solution of Eq. (7) shown in blue (solid), an approximate MAT solution given by Eq. (32) shown in red (dashed), and the leading eigenvalue solution given by Eq. (33) shown in green (dotted) for a suite of uniform-to-uniform transitions involving diffusion-only, diffusion-death, and advection-diffusion processes, respectively. For all problems we consider an initial condition $C_0(x) = 1$ on $0 \leqslant x \leqslant 50$, with $C(0,t) = 0$ and $C(50,t) = 0$ giving $C_\infty(x) = 0$. The diffusion-only results in (a, b) correspond to $(D = 0.5, V = 0, k = 0)$, the diffusion-death results in (c, d) correspond to $(D = 0.5, V = 0, k = 0.005)$, and the advection-diffusion results in (e, f) correspond to $(D = 0.5, V = 0.1, k = 0)$. Profiles in (a), (c), and (e) compare the three solutions at position $x = 10$, while profiles in (b), (d), and (f) compare the three solutions at position $x = 25$. The corresponding value of $T(x)$ is shown with a vertical line in all subfigures. Numerical results are obtained using the same technique outlined in the main text with $\delta x = 0.05$ and $\delta t = 0.1$.

With the appropriate boundary conditions for Eq. (36), $T(0) = T(L) = 0$, the solution can be written as

$$T(x) = Ae^{m^+ x} + Be^{m^- x} + \frac{n}{k}, \tag{39}$$

where

$$m^\pm = \frac{V}{2D} \pm \sqrt{\left(\frac{V}{2D}\right)^2 + \frac{k}{nD}}, \quad A = \frac{n(\mathrm{e}^{m^- L} - 1)}{k(\mathrm{e}^{m^+ L} - \mathrm{e}^{m^- L})},$$
$$B = \frac{n(1 - \mathrm{e}^{m^+ L})}{k(\mathrm{e}^{m^+ L} - \mathrm{e}^{m^- L})}. \tag{40}$$

We examine the effectiveness of our approximate solution for $T(x)$ for Eq. (35) in Fig. 5 on $0 \leqslant x \leqslant 50$ with $C(0,t) = 0$, $C(50,t) = 0$, $C_0(x) = 1$, and $C_\infty(x) = 0$. Numerical solutions of Eq. (35) are obtained with the same finite difference algorithm used for the linear problem, except that Picard linearization, with an absolute convergence tolerance of $1 \times 10^{-6}$, is used to solve the resulting systems of nonlinear equations [24]. Numerical solutions of Eq. (35) are shown in Figs. 5(a), 5(c), 5(e), and 5(g), where we see that the profiles evolve toward $C_\infty(x) = 0$ faster as $n$ decreases, as expected. Results in Figs. 5(b), 5(d), 5(f), and 5(h) compare the solution of the approximate equation for $T(x)$ [Eq. (39)] with a numerical approximation of the exact expression [Eq. (2)]. In accordance with our observations about the transient solution, we see that the MAT increases with $n$. Furthermore, we see that our approximate expression for the MAT gives an exact result when $n = 1$, as expected. More importantly, we obtain a good approximation when the governing equation is nonlinear and $n \neq 1$. We see that our approximation is an underestimate of the true MAT and that the accuracy of the approximation depends on $n$, since the profile for $n = 2$ is more accurate than the profile with $n = 3$.

## VI. DISCUSSION AND CONCLUSION

Estimating the critical time of a particular advection-diffusion-reaction process is fundamental for many applications in the physical sciences. In 2010–2011 Berezhkovskii introduced the concept of LAT to provide an estimate of the time required for a morphogen gradient to develop by studying the solution of a reaction-diffusion equation in the context of the development of the *drosophila* wing disk [7–9]. In our work, we have reexamined Berezhkovskii's recent definition of LAT and shown that it is identical to McNabb's 1991 definition of MAT. Previous analyses of MAT have been limited to diffusive systems, and we have extended these previous studies by considering the MAT for a general one-dimensional linear advection-diffusion-reaction equation. Therefore, our work can be used to estimate the critical time for a general linear advection-diffusion-reaction process.

Our work was motivated, in part, by seeking to provide physical insight into the meaning of MAT. We note that

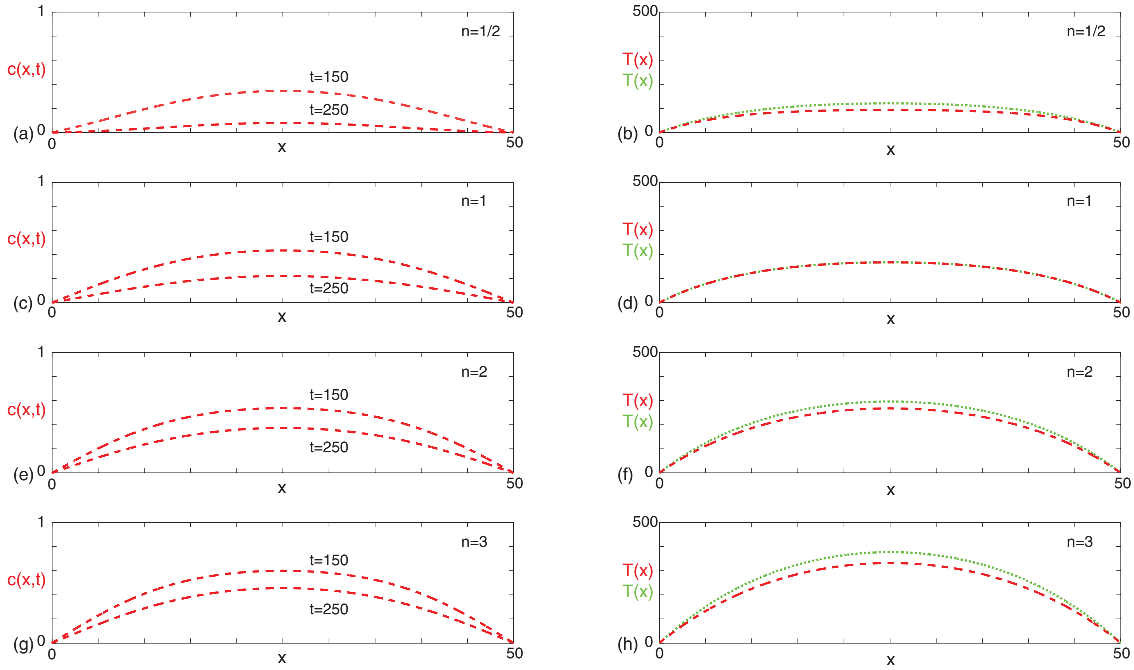


FIG. 5. (Color online) MAT for nonlinear diffusion reaction [Eq. (35) with $D = 0.5, V = 0, k = 0.005$] for a uniform-to-uniform transition on $0 \leqslant x \leqslant 50$ with $C(0,t) = 0$, $C(50,t) = 0$, $C_0(x) = 1$, and $C_\infty(x) = 0$. Results in (a, b), (c, d), (e, f), and (g, h) are for $n = 1/2,1,2,3$, respectively. Profiles in the left column show the solution of Eq. (35) at $t = 150$ and $t = 250$, as indicated. Results in the right column show the exact solution of the approximate model for the nonlinear MAT in red (dashed) and a numerical approximation of Eq. (2) in green (dotted). All numerical results are obtained using the same technique outlined in the main text with $\delta x = 0.05$ and variable $\delta t$ with $1 \times 10^{-5} \leqslant \delta t \leqslant 1$. The numerical solution of Eq. (35) is obtained with Picard linearization with absolute convergence tolerance $1 \times 10^{-6}$.

McNabb introduced the concept of MAT by considering a simple linear ode model [Eq. (14)] and he stated that the MAT for this model corresponds to the MPLT for the underlying stochastic death process. To build on this initial work, we further explored the connection between MAT and MPLT by examining the relationship between MAT and MPLT for a range of spatial linear transport problems governed by a linear advection-diffusion-reaction equation. We used a combination of continuum and discrete approaches to study the MAT and MPLT for both uniform-to-uniform transitions and nonuniform transitions. In all cases, including diffusive transport, combined diffusion-death processes, and combined diffusion-advection transport, our results indicate that the MAT and MPLT are identical only for uniform-to-uniform transitions. Our work shows that MAT and MPLT are not equivalent for more general nonuniform transitions.

We sought to examine an approximation introduced by Berezhkovskii [7] where the exact solution of a pde model was approximated by an exponential solution based on the MAT. Comparing Berezhkovskii's exponential solution, a leading eigenvalue approximate solution and the full numerical solution for several uniform-to-uniform transition problems shows that the accuracy of Berezhkovskii's exponential solution is problem dependent. This observation means that it is difficult to distinguish between situations where the exponential solution provides a useful approximation from other situations where the exponential solution is a poor approximation.

Most of the analysis presented in our work is relevant for the linear advection-diffusion-reaction equation. Evaluating the MAT for a linear process is greatly simplified because the boundary value problem for the MAT does not explicitly depend on the solution of the underlying linear equation. Of course, estimating critical times for nonlinear advection-diffusion-reaction processes is also of great interest across many disciplines in the physical sciences. Calculating the MAT for a nonlinear equation is more challenging, since the boundary value problem for the MAT depends explicitly on the solution of the underlying nonlinear equation. While this complication does not impede a numerical approximation of the MAT, to provide analytical insight some approximation must be introduced. We address this by proposing an approximate boundary value problem for $T(x)$ when the decay term is nonlinear. Exact solutions of the approximate boundary value problem are presented, and we show that these solutions provide a simple and useful approximation to the numerical MAT profile that was generated using the exact governing equations without any assumptions. Our future work aims to develop additional approximations and to apply them to physical processes that are governed by other nonlinear advection-diffusion-reaction equations.

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