Particle lifetime in cylindrical cavity with absorbing spot on the wall: Going beyond the narrow escape problem

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The mean lifetime of a particle diffusing in a cylindrical cavity with a circular absorbing spot on the cavity wall is studied analytically as a function of the spot radius, its location on the wall, the particle initial position, and the cavity shape determined by its length and radius. When the spot radius tends to zero our formulas for the mean lifetime reduce to the result given by the solution of the narrow escape problem, according to which the mean lifetime is proportional to the ratio of the cavity volume to the spot radius and is independent of the cavity shape, the spot location on the cavity wall, and the particle starting point, assuming that this point is not too close to the spot. When the spot radius is not small enough, the asymptotic narrow escape formula for the mean lifetime fails, and one should use more general formulas derived in the present study. To check the accuracy and to establish the range of applicability of the formulas, we compare our theoretical predictions with the results of Brownian dynamics simulations. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4772183>]

I. INTRODUCTION

This paper deals with trapping of diffusing particles in a cavity by an absorbing circular spot on the wall. The focus is on the mean particle lifetime. This lifetime plays an important role in the analysis of diffusive transport in different compartmentalized systems. Examples include transport in spiny dendrites,¹ endosomal sorting,² controlled drug delivery,³ channel-facilitated membrane transport,⁴ transport in porous media and materials,⁵ etc. Under certain conditions, which are discussed below, the mean particle lifetime τ in a cavity of volume V is given by

$$\tau = \frac{V}{4Da}, \quad (1.1)$$

where a is the spot radius, and D is the particle diffusion constant. According to Eq. (1.1), τ is independent of the cavity shape and depends only on its volume. In addition, τ is independent of both the spot location on the cavity wall and the particle initial position. The expression in Eq. (1.1) is applicable when the spot is small enough, so that (i) it can be considered as a perfectly absorbing disk on a locally flat surface, and (ii) the particle mean first passage time to the spot significantly exceeds the relaxation time in the cavity. The latter implies that the particle starting point must be sufficiently far away from the spot. One can find rigorous derivation of the expression for τ in Eq. (1.1) in the papers cited in Ref. 6. Its back-of-the-envelope derivation and numerical test can be found in Ref. 7.

A heuristic derivation of Eq. (1.1) is as follows.⁷ Consider a circular disk of radius a on a flat wall and point particles diffusing in the semi-space outside the wall. As soon as a particle touches the disk, both instantly annihilate. When the

particle concentration c is low enough, the survival probability of the disk for time t , $S_d(t)$, decays as a single exponential,

$$S_d(t) = e^{-k_H ct}, \quad (1.2)$$

where k_H is the Hill rate constant given by⁸

$$k_H = 4Da. \quad (1.3)$$

Next consider the same disk on a locally flat surface of a large cavity of volume V containing the only particle. In this case, the particle concentration is equal to $1/V$, and the disk survival probability is equal to that of the particle, which we denote by $S(t)$. If the particle starts sufficiently far away from the disk, the search time significantly exceeds the particle equilibration time in the cavity, and the annihilation kinetics is single exponential,

$$S(t) = S_d(t) = e^{-k_H t / V}, \quad (1.4)$$

where we have used Eq. (1.2) with $c = 1/V$. According to Eq. (1.4), the probability density of the particle lifetime, $\varphi(t)$, is given by

$$\varphi(t) = -\frac{dS(t)}{dt} = \frac{k_H}{V} e^{-k_H t / V}. \quad (1.5)$$

Then the mean lifetime of the particle is

$$\tau = \int_0^\infty t \varphi(t) dt = \int_0^\infty S(t) dt = \frac{V}{k_H}. \quad (1.6)$$

Substituting here k_H given in Eq. (1.3) we arrive at the result for τ in Eq. (1.1).

The problem of the particle trapping by a perfectly absorbing disk is, in fact, the problem of the first passage time

FIG. 1. Schematic representation of a cylindrical cavity of radius R and length L with a circular absorbing spot of radius a on the cavity wall. The spot is in the center of the end wall in panel (a) and on the sidewall in panel (b).

of the particle to the disk. When the disk is small, this is the so-called narrow escape problem. In the present paper we go beyond the narrow escape problem in the special case of a cylindrical cavity.

We consider two different locations of the spot on the cavity wall, shown in panels (a) and (b) of Fig. 1, and derive formulas for the mean particle lifetime, which contain the result in Eq. (1.1) as a special limiting case. For the spot located at the cavity end wall (Fig. 1(a)), the formula in Eq. (2.7) gives the mean lifetime not only for small but also for arbitrary spot radius, including the situation where the spot occupies the entire end wall. When the spot is located on the sidewall (Fig. 1(b)), the formula in Eq. (3.8) gives the mean lifetime for an arbitrary location of the spot on the sidewall. The formulas in Eqs. (2.7) and (3.8) give the mean lifetime as functions of the particle initial position in the cavity. In addition, these formulas show how the mean lifetime depends on the spot location on the cavity surface.

The key step of our analysis is the replacement of the initial three-dimensional problem by an effective one-dimensional one. This replacement is not rigorous. Therefore, our analytical results do not provide an exact solution to the problem. To check the accuracy of our approximate theory and to establish the range of its applicability, we compare our analytical results with those obtained from Brownian dynamics simulations.

The outline of the paper is as follows. The geometries shown in panels (a) and (b) of Fig. 1 are considered in Secs. II and III, respectively. Finally, some concluding remarks are made in Sec. IV.

II. ABSORBING SPOT AT THE CAVITY END WALL

Consider a point particle diffusing in a cylindrical cavity of radius R and length L with a perfectly absorbing circular spot of radius a , $0 < a \leq R$, located in the center of the cavity end wall as shown in Fig. 1(a). Initially ($t = 0$), the particle is uniformly distributed over the cavity cross section $x = x_0$, where the x -coordinate measures the particle position along

the cavity axis, $0 \leq x, x_0 \leq L$. The particle propagator in the x -direction (the Green's function), $G(x, t|x_0)$, satisfies the diffusion equation,

$$\frac{\partial G}{\partial t} = D \frac{\partial^2 G}{\partial x^2}, \quad 0 < x < L, \quad (2.1)$$

subject to the initial condition $G(x, 0|x_0) = \delta(x - x_0)$, as well as reflecting and partially absorbing boundary conditions at $x = 0$ and $x = L$, respectively,

$$\left. \frac{\partial G}{\partial x} \right|_{x=0} = 0, \quad - \left. \frac{\partial G}{\partial x} \right|_{x=L} = \kappa G|_{x=L}. \quad (2.2)$$

The trapping rate κ entering into the boundary condition at the cavity end wall containing the absorbing spot can be obtained by homogenization of the boundary. In the case under consideration κ is given by⁹

$$\kappa = \frac{4Da}{\pi R^2} f(\nu), \quad (2.3)$$

where $\nu = a/R$, $0 < \nu \leq 1$, and function $f(\nu)$ is

$$f(\nu) = \frac{1 + 1.37\nu - 0.37\nu^2}{(1 - \nu^2)^2}. \quad (2.4)$$

This function monotonically increases with ν from unity at $\nu = 0$ to infinity as $\nu \rightarrow 1$. Respectively, κ monotonically increases from $4Da/(\pi R^2)$ at small a to infinity as a approaches R and the whole cavity end wall becomes perfectly absorbing.

Equations (2.1)–(2.4) provide a one-dimensional description of the three-dimensional trapping problem, which involves homogenization of the inhomogeneous boundary at the cavity end wall at $x = L$. One can find detailed discussion of boundary homogenization in Ref. 9 and papers cited therein.

When the particle motion is described by Eqs. (2.1) and (2.2), the mean lifetime of the particle starting from $x = x_0$ is the sum of its mean first-passage time from x_0 to the partially absorbing end of the interval, $\tau_{FP}(x_0 \rightarrow L)$, and its mean lifetime, conditional on that the particle starts from the partially absorbing end. The latter is given by L/κ , while the former is

$$\tau_{FP}(x_0 \rightarrow L) = \frac{L^2 - x_0^2}{2D}. \quad (2.5)$$

Thus, the mean lifetime of interest, $\tau_{ew}(x_0)$, is

$$\tau_{ew}(x_0) = \tau_{FP}(x_0 \rightarrow L) + \frac{L}{\kappa}, \quad (2.6)$$

where subscript “ew” indicates that the absorbing spot is located on the cavity end wall. The expression in Eq. (2.6) can be obtained by solving the equation $Dd^2\tau_{ew}(x_0)/dx_0^2 = -1$ subject to the boundary conditions $-Dd\tau_{ew}(x_0)/dx_0|_{x_0=L} = \kappa\tau_{ew}(L)$ and $d\tau_{ew}(x_0)/dx_0|_{x_0=0} = 0$. Using the expression for κ in Eq. (2.3), we can write Eq. (2.6) as

$$\tau_{ew}(x_0) = \frac{L^2 - x_0^2}{2D} + \frac{V}{4Da f(\nu)}, \quad (2.7)$$

where $V = \pi R^2 L$ is the cavity volume. This is one of the main results of the present study. The expression in Eq. (2.7) reduces to the narrow escape result for the mean lifetime, Eq. (1.1), when (i) the first term in Eq. (2.7) can be neglected, i.e., the cavity length L is not too large, and (ii) $a \ll R$, so that $\nu \ll 1$ and $f(\nu) \approx 1$.

FIG. 2. The ν -dependences of the mean particle lifetime given by Eq. (2.10) with $x_0 = 0$ and $L/R = 1, 2, 4, 6, 8$, and 10 (solid curves) and obtained from Brownian dynamics simulations (symbols). The simulation results were obtained by averaging over 50 000 trajectories. The time step used in the simulations was $10^{-6}R^2/D$. The starting points of the trajectories were uniformly distributed over the cavity cross section $x_0 = 0$.

The ratio of $\tau_{ew}(x_0)$ to the asymptotic, narrow escape expression for the mean lifetime, Eq. (1.1), is

$$\frac{4Da\tau_{ew}(x_0)}{V} = \frac{2\nu(L^2 - x_0^2)}{\pi RL} + \frac{(1 - \nu^2)^2}{1 + 1.37\nu - 0.37\nu^4}. \quad (2.8)$$

This ratio is close to unity for all values of x_0 when

$$\nu \ll 1 \text{ and } L \ll \frac{R}{\nu} = \frac{R^2}{a}. \quad (2.9)$$

The first inequality guarantees that $f(\nu) \approx 1$ and the trapping rate is given by a simple formula $\kappa \approx 4Da/(\pi R^2)$. The second inequality constraints the cavity length, that, in turn, guarantees fast intra-cavity relaxation. If the inequalities are not fulfilled, $\tau_{ew}(x_0)$ deviates from its asymptotic value, so that the ratio $4Da\tau_{ew}(x_0)/V$ differs from unity (see Figs. 2–4).

The ν -dependences predicted by Eq. (2.8) are compared with the values of the ratio $4Da\tau_{ew}(x_0)/V$ obtained from Brownian dynamics simulations at three values of x_0 , $x_0 = 0$, $L/2$, and L , in Figs. 2–4, respectively. For these values of x_0 , Eq. (2.8) takes the form

$$\frac{4Da\tau_{ew}(x_0)}{V} = \frac{(1 - \nu^2)^2}{1 + 1.37\nu - 0.37\nu^4} + \frac{\nu L}{\pi R} \times \begin{cases} 2, & x_0 = 0 \\ 1.5, & x_0 = L/2 \\ 0, & x_0 = L \end{cases} \quad (2.10)$$

We compare this with numerical results for $L/R = 1, 2, 4, 6, 8$, and 10 at $x_0 = 0$ and $x_0 = L/2$ in Figs. 2 and 3. When $x_0 = L$, the ratio $4Da\tau_{ew}(x_0)/V$ is independent of L . In Fig. 4 we compare the ν -dependence predicted by Eq. (2.10) at $x_0 = L$ with the numerical results obtained for the cavity of length $L = 10R$. These results are indistinguishable from those obtained for cavities of other lengths. One can see excellent agreement between the theoretical predictions and numerical results shown in Figs. 2–4.

FIG. 3. The ν -dependences of the mean particle lifetime given by Eq. (2.10) with $x_0 = L/2$ and $L/R = 1, 2, 4, 6, 8$, and 10 (solid curves) and obtained from Brownian dynamics simulations (symbols). The simulation results were obtained by averaging over 50 000 trajectories. The time step used in the simulations was $10^{-6}R^2/D$. The starting points of the trajectories were uniformly distributed over the cavity cross section $x_0 = L/2$.

Let $\langle \tau_{ew} \rangle$ be the mean lifetime averaged over the uniform distribution of the particle starting point in the cavity,

$$\langle \tau_{ew} \rangle = \frac{1}{L} \int_0^L \tau_e(x_0) dx_0. \quad (2.11)$$

Averaging the ratio given in Eq. (2.8) we obtain

$$\frac{4Da\langle \tau_{ew} \rangle}{V} = \frac{4\nu L}{3\pi R} + \frac{(1 - \nu^2)^2}{1 + 1.37\nu - 0.37\nu^4}. \quad (2.12)$$

This ν -dependence is compared with the values of $4Da\langle \tau_{ew} \rangle / V$ obtained from Brownian dynamics simulations for $L/R = 1, 2, 4, 6, 8$, and 10 in Fig. 5. One can see that the

FIG. 4. The ν -dependence of the mean particle lifetime given by Eq. (2.10) with $x_0 = L$ and $L/R = 10$ (solid curve) and obtained from Brownian dynamics simulations (symbols). The simulation results were obtained by averaging over 50 000 trajectories. The time step used in the simulations was $10^{-6}R^2/D$. The starting points of the trajectories were uniformly distributed over the cavity cross section $x_0 = L$.

FIG. 5. The ν -dependences of the mean particle lifetime averaged over the particle initial position given by Eq. (2.12) with $L/R = 1, 2, 4, 6, 8$, and 10 (solid curves) and obtained from Brownian dynamics simulations (symbols). The simulation results were obtained by averaging over 50 000 trajectories. The time step used in the simulations was $10^{-6}R^2/D$. The starting points of the trajectories were uniformly distributed over the cavity volume.

ν -dependences predicted by Eq. (2.12) for different values of L/R are in perfect agreement with the numerical results.

III. ABSORBING SPOT ON THE CAVITY SIDEWALL

In this section we consider a point particle diffusing in the same cylindrical cavity of radius R and length L with a small perfectly absorbing circular spot of radius a , $a \ll R$, which is now located on the sidewall of the cavity at distance x_a from its left end located at $x = 0$ (Fig. 1(b)). The one-dimensional propagator of the particle starting from the cross section $x = x_0$, in this case, satisfies the diffusion equation with a sink term,

$$\frac{\partial G}{\partial t} = D \frac{\partial^2 G}{\partial x^2} - \gamma \delta(x - x_a)G, \quad 0 < x < L, \quad (3.1)$$

subject to the initial condition $G(x, 0|x_0) = \delta(x - x_0)$ and reflecting boundary conditions at the ends of the interval,

$$\left. \frac{\partial G}{\partial x} \right|_{x=0, L} = 0. \quad (3.2)$$

The sink term describes trapping of the particle by the absorbing spot. Using the fact that $a \ll R$, we approximate the sink by a delta function with the sink intensity γ given by¹⁰

$$\gamma = \frac{4Da}{\pi R^2}. \quad (3.3)$$

The mean lifetime $\tau_{sw}(x_0, x_a)$ of a particle diffusing on an interval of length L , $0 < x < L$, which starts from $x = x_0$ and is trapped by a delta sink of intensity γ located at $x = x_a$, is given by

$$\tau_{sw}(x_0, x_a) = \tau_{FP}(x_0 \rightarrow x_a) + \frac{L}{\gamma}, \quad (3.4)$$

where subscript “sw” indicates that the absorbing spot is on the sidewall, and $\tau_{FP}(x_0 \rightarrow x_a)$ is the mean first-passage time from the starting point $x = x_0$ to the point $x = x_a$ where the

sink is located. Note that the expression for the mean lifetime in Eq. (2.6) is a special case of the expression in Eq. (3.4) corresponding to $x_a = L$ and $\gamma = \kappa$. This is a consequence of the fact that a delta sink of intensity κ located near the reflecting boundary at $x = L$ is equivalent to the partially absorbing boundary of the interval. The expression in Eq. (3.4) has the same interpretation as the expression in Eq. (2.6). To be absorbed by the sink, the particle has to reach point x_a . $\tau_{FP}(x_0 \rightarrow x_a)$ is the mean time required for that. The second term in the right-hand side of Eq. (3.4), L/γ , is the mean lifetime of the particle that starts from point x_a , i.e., $x_0 = x_a$. Using Eq. (3.3), we can write the mean lifetime in Eq. (3.4) as

$$\tau_{sw}(x_0, x_a) = \tau_{FP}(x_0 \rightarrow x_a) + \frac{V}{4Da}. \quad (3.5)$$

The second term on the right-hand side of Eq. (3.5) is identical to the asymptotic narrow escape result for the mean lifetime, Eq. (1.1). Thus, the expression in Eq. (1.1) provides a good approximation for the mean lifetime when the inequality

$$\tau_{FP}(x_0 \rightarrow x_a) \ll \frac{V}{4Da} \quad (3.6)$$

is fulfilled, and the first term on the right-hand side of Eq. (3.5) can be neglected. The mean first passage time $\tau_{FP}(x_0 \rightarrow x_a)$ is given by

$$\tau_{FP}(x_0 \rightarrow x_a) = \begin{cases} \frac{x_a^2 - x_0^2}{2D}, & 0 \leq x_0 \leq x_a \\ \frac{(x_0 - x_a)(2L - x_0 - x_a)}{2D}, & x_a \leq x_0 \leq L \end{cases}. \quad (3.7)$$

The requirement that the inequality, Eq. (3.6), is fulfilled at arbitrary starting point of the particle sets a limit on the length L of the cavity. This requirement is equivalent to that of fast intra-cavity relaxation compared to the mean lifetime.

When the cavity is long, and the inequality, Eq. (3.6), can be violated, both terms on the right-hand side of Eq. (3.5) must be taken into account. As a result, the mean first passage time becomes a function of both the initial position of the particle, x_0 , and the spot location on the cavity wall, x_a . Substituting $\tau_{FP}(x_0 \rightarrow x_a)$ given in Eq. (3.7) into Eq. (3.5) we arrive at

$$\begin{aligned} \tau_{sw}(x_0, x_a) &= \begin{cases} \frac{x_a^2 - x_0^2}{2D} + \frac{V}{4Da}, & 0 \leq x_0 \leq x_a \\ \frac{(x_0 - x_a)(2L - x_0 - x_a)}{2D} + \frac{V}{4Da}, & x_a \leq x_0 \leq L \end{cases}. \end{aligned} \quad (3.8)$$

This is the second main result of the present study.

In the rest of this section the focus is on the mean lifetime dependence on the spot location on the cavity sidewall. With this in mind we introduce $\langle \tau_{sw}(x_a) \rangle$, which is the mean lifetime $\tau_{sw}(x_0, x_a)$, Eq. (3.8), averaged over the particle starting

TABLE I. Relative error of the theoretical predictions, Eq. (3.11), in percent as a function of the distance from the center of the absorbing spot to the nearest cavity end wall for cavities of various lengths, $L = R$, $2R$, and $4R$.

x_a/R	x_a/a	$L = R$	$L = 2R$	$L = 4R$
2	40			<1
1	20			<1
0.5	10	<1	<1	<1
0.25	5	2.02	2.29	2.37
0.125	2.5	7.91	8.90	6.00
0.0625	1.25	18.08	19.67	17.17

point x_0 ,

$$\langle \tau_{sw}(x_a) \rangle = \frac{1}{L} \int_0^L \tau_{sw}(x_0, x_a) dx_0. \quad (3.9)$$

Carrying out the integration we arrive at

$$\langle \tau_{sw}(x_a) \rangle = \frac{L^2}{D} \left[\frac{1}{12} + \left(\frac{x_a}{L} - \frac{1}{2} \right)^2 \right] + \frac{V}{4Da}. \quad (3.10)$$

This shows how the averaged mean lifetime depends on the spot location on the sidewall of the cavity.

To check the accuracy of our approximate theory and to establish the range of its applicability, we compare the averaged mean lifetime predicted by Eq. (3.10) with the values of $\langle \tau_{sw}(x_a) \rangle$ obtained from Brownian dynamics simulations. We define the relative error of the theoretical predictions as

$$\left| \frac{\langle \tau_{sw}(x_a) \rangle_{theory}}{\langle \tau_{sw}(x_a) \rangle_{simulations}} - 1 \right|, \quad (3.11)$$

where $\langle \tau_{sw}(x_a) \rangle_{theory}$ and $\langle \tau_{sw}(x_a) \rangle_{simulations}$ are the mean lifetimes, averaged over the particle starting point, given by Eq. (3.10) and obtained from simulations, respectively. The relative errors were found for different values of the distance x_a from the center of the absorbing spot of radius $a = 0.05R$ ($\nu = 0.05$) to the nearest end wall in cavities of lengths, $L = R$, $2R$, and $4R$. These relative errors are given in Table I.

One can see that the relative error of the theoretical predictions depends on the distance from the spot center to the nearest cavity end wall. The relative error is less than 2.5% when $x_a \geq 5a$. At smaller distances the theory underestimates the averaged mean lifetime. Presumably, this is a consequence of the fact that the delta-function approximation of the absorbing spot fails when the spot approaches the cavity end wall. Then this is not surprising that the relative error is about 9% and 20% when the distance from the spot center to the nearest cavity end wall is $x_a = 2.5a$ and $x_a = 1.25a$, respectively.

IV. CONCLUDING REMARKS

In the present paper we have studied trapping of a particle diffusing in a cylindrical cavity by a circular absorbing spot on the cavity wall, focusing on the mean particle lifetime. When the spot radius tends to zero, this is the narrow escape problem, in which the mean lifetime, Eq. (1.1), is independent of the cavity shape, the spot location on the cavity wall, and the particle starting point, assuming that this point is not too close to the spot. The goal of this study is to develop

a theory that goes beyond the narrow escape problem in the sense that it provides a solution, which shows how the mean lifetime depends on the cavity shape, the spot location on the cavity wall, and the particle starting point. Such a theory has been developed for the special case of a cylindrical cavity.

Our main results are the expressions for the mean lifetime in Eqs. (2.7) and (3.8). The former gives the mean lifetime in the situation where the spot is located in the center of the cavity end wall as shown in Fig. 1(a). The spot radius can be arbitrary, including the limiting case where the spot occupies the entire end wall and its radius is equal to the cavity radius. The expression in Eq. (3.8) gives the mean lifetime in the case where the spot is located on the sidewall of the cavity shown in Fig. 1(b), assuming that the spot radius is small compared to both the cavity length and radius.

To discuss the range of applicability of these results, we note that their derivations are based on the effective one-dimensional formulations of the initial three-dimensional problems. In deriving Eq. (2.7), we used boundary homogenization to describe trapping by the spot located in the center of the cavity end wall. As shown in Ref. 11, in this case boundary homogenization is applicable at arbitrary radius of the absorbing spot when the length of the cavity is larger than its radius, $R < L$. In deriving Eq. (3.8), we used delta sink to describe trapping by a small spot located on the cavity sidewall. Our analysis has shown that the obtained results are applicable when the distance from the spot center to the nearest cavity end exceeds five spot radii, since the delta sink approximation fails when the spot center approaches the end wall of the cavity. Since the approach we use to find the solution is based on the intuitively appealing replacement of the initial three-dimensional problem by an equivalent one-dimensional one, our analytical results do not provide an exact solution to the problem.

To summarize, when the spot is small, Eqs. (2.7) and (3.8) show how the mean particle lifetime depends on both the particle starting point and the spot location on the cavity wall. In addition, when the spot is located in the center of the cavity end wall, Eq. (2.7) gives the mean lifetime as a function of the spot radius not only for small spots, but over the whole range of the radius, including the case where the spot occupies the entire end wall and the spot radius is equal to that of the cavity.

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