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The problem of trapping of diffusing particles by identical, perfectly absorbing rings periodically distributed along an otherwise reflecting infinite cylindrical tube is very difficult for analytical treatment due to the mixed boundary conditions on the tube surface. Analytical solutions to this problem are considered in two recent papers.[1,2] Among other results reported in these works, the authors propose approximate expressions for the mean lifetime τ of a particle whose starting point is uniformly distributed over the tube surface, and the tube is surrounded by an outer concentric tube which is a reflecting boundary for diffusing particles. These expressions can be written in a unified form as

$$\tau = \left[L\left(R^2 - \rho^2\right)/(2\pi D\rho)\right] f, \tag{1}$$

where ρ and L are the radius and half-period of the inner tube, R is the outer tube radius, and D is the particle diffusivity. The factor f is, in general, a dimensionless function of three dimensionless geometric parameters: ρ/L, R/L, and $\varepsilon = \pi l/L$, where l is the half-width of the absorbing ring, and hence, l/L is the surface fraction of the inner tube covered by the rings. The two papers give different expressions for this factor, denoted by f_1 and f_2. In this note, these expressions are tested against exact values of f obtained by solving the mixed boundary-value problem numerically by the finite element method.

Being motivated by search problems in biology, the authors of Ref. 1 studied the binding of a particle diffusing inside a finite-length outer cylinder (a "bacillus-shaped bacteria") to a partially absorbing ring located on the surface of a concentric inner cylinder in the geometry shown in Fig. 1. Such trapping problems arise, for example, in modeling protein binding to specific sequences on DNA molecules or on specific locations of the nucleolus that generates cascades of biochemical reactions that support the functioning of living systems.[3–8] The focus of Ref. 1 is on the mean particle lifetime considered as a function of the particle initial position, geometric parameters of the system, the intrinsic reactivity of the ring surface, and the particle diffusivity. To solve the problem, the authors adopt the approximate approach proposed in Ref. 9. This allows them to obtain an analytical expression for the mean lifetime. In the special case where the ring is perfectly absorbing and the particle starting point is uniformly distributed over the surface of the inner cylinder, their general result reduces to the expression for τ in Eq. (1) with the factor f given by

$$f \approx f_1 = 2\sum_{n=1}^{\infty} (G_n/n)[\sin n\varepsilon/(n\varepsilon)]^2, \tag{2}$$

with

$$G_n = \frac{I_1(\pi nR/L)K_0(\pi n\rho/L) + I_0(\pi n\rho/L)K_1(\pi nR/L)}{I_1(\pi n\rho/L)K_1(\pi nR/L) - I_1(\pi nR/L)K_1(\pi n\rho/L)}, \tag{3}$$

where $I_\nu(z)$ and $K_\nu(z)$ are the modified Bessel functions of the first and second kind.

By symmetry, the trapping problem analyzed in Ref. 1 is equivalent to that in the case of two infinite concentric cylindrical tubes

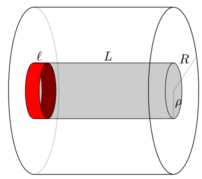

FIG. 1. Schematic view of the diffusion domain studied in Ref. 1. A particle diffuses between the two concentric cylinders of radii R and $\rho \le R$. The intercylinder space is constrained by two reflecting walls separated by distance L, which are perpendicular to the cylinder axis. The particle is trapped by a partially absorbing ring of length l located on the inner cylinder near the reflecting wall. The rest of the inner cylinder surface and that of the outer cylinder are reflective.

with partially absorbing rings of width $2l$ periodically arranged on the inner tube, with period $2L$. Trapping by infinite periodically striped cylindrical surfaces is studied in Ref. 2, assuming that the stripes are perfectly absorbing. The analysis is performed for three orientations of the stripe direction with respect to the tube axes: perpendicular, parallel, and at the angle $\pi/4$ to the axis. This is done for both internal and external problems, where the particles diffuse inside and outside the striped tube, respectively. The key approximation used in Ref. 2 is the so-called boundary homogenization which is the replacement of nonuniform boundary conditions on the surface by an effective radiation boundary condition with properly chosen reactivity that is uniform over the surface. Since a striped cylindrical surface can be formed by "rolling" a corresponding flat striped surface, it is hypothesized that its reactivity is the same as that of the flat surface, for which the effective surface reactivity is known.[10] For the mean particle lifetime discussed above, this leads to the expression for τ in Eq. (1) with the factor f given by

$$f \approx f_2 = 2\ln(1/\sin(\varepsilon/2)), \tag{4}$$

which is much simpler than its counterpart in Eq. (2). In contrast to the factor f_1, the factor f_2 depends only on $\varepsilon = \pi l/L$, i.e., on the strip surface fraction, and is independent of two other parameters, ρ/L and R/L. Note that f_1 and f_2 have the same asymptotic behavior in the limiting case of $\varepsilon \to 0$, where the strip width tends to zero, and both expressions for the factor f diverge as $2\ln(1/\varepsilon)$. As might be expected, both f_1 and f_2 vanish when $\varepsilon \to \pi$ since the entire inner tube surface becomes absorbing.

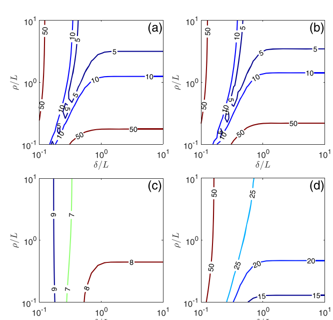

FIG. 2. Contour plots showing the absolute values of the relative error of the two approximate expressions for the factor f, given in Eqs. (2) and (4), in percent, $100|1 - f_i/f|$, $i = 1, 2$, as functions of the geometric parameters $\delta = R - \rho$ and ρ, where δ is the distance between the inner and outer cylinders, rescaled by the system length L. The contour plots are presented for two values of the surface fraction occupied by the absorbing ring on the inner cylinder, $l/L = 0.1$ [panels (a) and (c)] and $l/L = 0.5$ [panels (b) and (d)]. The relative errors of Eqs. (4) and (2) are shown in panels (a) and (b) and panels (c) and (d), respectively. The numbers indicate the magnitudes of the relative error.

Below we compare the expressions in Eqs. (2) and (4) with the exact solution for the factor f obtained numerically with the aim to establish their accuracy and limitations. This is done for a wide range of inner and outer tube radii at two values of the ring surface fraction, when the rings occupy one tenth and one half of the inner tube surface, $\varepsilon = \pi/10$ and $\varepsilon = \pi/2$, respectively. The results of the comparison are presented in Fig. 2 that shows the contour plots of the absolute values of the relative error of the two expressions in percent, $100|1 - f_i/f|$, $i = 1, 2$, as functions of δ/L and ρ/L, where $\delta = R - \rho$ is the distance between the inner and outer tubes. The relative error of Eq. (4) is shown in panels (a) and (b) for $l/L = 0.1$ and 0.5, respectively. Corresponding results for Eq. (2) are presented in panels (c) and (d). As ρ/L and δ/L tend to infinity, the relative errors approach their asymptotic values. For the expression in Eq. (4), this asymptotic value is zero (by construction) since the cylindrical geometry becomes effectively flat in this limiting case. The asymptotic value of the relative error of the expression in Eq. (2) is a function of ε: it is 8% at $\varepsilon = \pi/10$ and about 20% at $\varepsilon = \pi/2$. From Fig. 2, one can see that the simple expression in Eq. (4) fails for narrow—compared to the system period $2L$—inner cylinders and when the outer tube is too close to the inner one—the distance δ is shorter or equal to the period $2L$. Otherwise, i.e., when both ρ and δ exceed $2L$, this expression accurately predicts the factor f. This is true for both values of the ring surface fraction. It is important that when Eq. (4) does not work, at small l/L, one can use Eq. (2) that predicts the factor f with high accuracy over the entire range of both parameters, ρ/L and δ/L, provided that the ring surface fraction is low.

To summarize, the expression for the factor f in Eq. (2) works better than its counterpart in Eq. (4) at small ring surface fractions. For example, at $l/L = 0.1$, the relative error of its predictions is less than 10% over the entire range of ρ/L and δ/L. As might be expected, this relative error increases with the ring surface fraction, but even at $l/L = 0.5$, it does not exceed 50%. As concerns the simple expression in Eq. (4), it is reliably applicable at an arbitrary ring surface fraction on condition that both ρ/L and δ/L are greater than unity. These two approximations complement each other.

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