Evaluating diffusion resistance of a constriction in a membrane channel by the method of boundary homogenization

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In this paper we analyze diffusive transport of noninteracting electrically uncharged solute molecules through a cylindrical membrane channel with a constriction located in the middle of the channel. The constriction is modeled by an infinitely thin partition with a circular hole in its center. The focus is on how the presence of the partition slows down the transport governed by the difference in the solute concentrations in the two reservoirs separated by the membrane. It is assumed that the solutions in both reservoirs are well stirred. To quantify the effect of the constriction we use the notion of diffusion resistance defined as the ratio of the concentration difference to the steady-state flux. We show that when the channel length exceeds its radius, the diffusion resistance is the sum of the diffusion resistance of the cylindrical channel without a partition and an additional diffusion resistance due to the presence of the partition. We derive an expression for the additional diffusion resistance as a function of the tube radius and that of the hole in the partition. The derivation involves the replacement of the nonpermeable partition with the hole by an effective uniform semipermeable partition with a properly chosen permeability. Such a replacement makes it possible to reduce the initial three-dimensional diffusion problem to a one-dimensional one that can be easily solved. To determine the permeability of the effective partition, we take advantage of the results found earlier for trapping of diffusing particles by inhomogeneous surfaces, which were obtained with the method of boundary homogenization. Brownian dynamics simulations are used to corroborate our approximate analytical results and to establish the range of their applicability.

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I. INTRODUCTION

Consider diffusion transport of electrically uncharged solute molecules through a membrane channel connecting two reservoirs separated by the membrane. We will assume that the solute molecules are point particles and that the transport is governed by the difference in the solute concentrations on the two sides of the membrane, denoted by Δc. When the solutions in both reservoirs are well stirred, and the solute molecules do not interact with each other inside the channel, the steady-state solute flux J through the channel is proportional to Δc and can be written as

$$J = \frac{\Delta c}{R_{\rm dif}}, \tag{1.1}$$

where $R_{\rm dif}$ is the channel diffusion resistance [1]. For a cylindrical channel of length L and radius a, this flux is given by

$$J_{\rm cyl} = \pi a^2 D \frac{\Delta c}{L}, \tag{1.2}$$

where D is the solute diffusivity in the channel, and hence the diffusion resistance, $R_{\rm dif}^{\rm cyl}$, is

$$R_{\rm dif}^{\rm cyl} = \frac{\Delta c}{J_{\rm cyl}} = \frac{L}{\pi a^2 D}. \tag{1.3}$$

This paper deals with the steady-state flux through a cylindrical channel of length L and radius a with an infinitely thin partition, located in the middle of the channel; the partition has a hole of radius b, $b < a$, in its center, as schematically shown in Fig. 1. The above relations, Eqs. (1.1)–(1.3), correspond to the case of no partition, where $a = b$. The presence of the partition slows down the transport. The focus is on how the slowdown depends on the geometric parameters of the system. To answer this question we derive approximate analytical expressions for the steady-state flux and diffusion resistance as functions of the geometric parameters a, b, and L,

$$J = \frac{\pi a^2 D}{L + \frac{\pi a^2}{2b} M(\xi)} \Delta c \tag{1.4}$$

and

$$R_{\rm dif} = \frac{\Delta c}{J} = \frac{L}{\pi a^2 D} + \frac{1}{2bD} M(\xi), \tag{1.5}$$

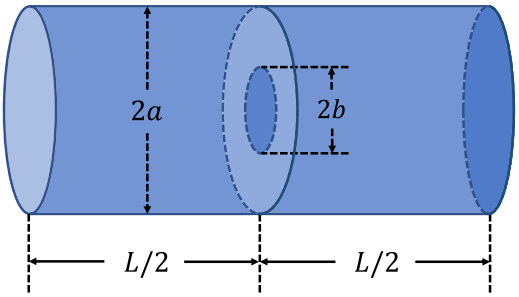

FIG. 1. Sketch of a cylindrical channel of length L and radius a with an infinitely thin partition, located in the middle of the channel; the partition has a hole of radius b, $b < a$, in its center.

where $\xi = b/a$ and function $M(\xi)$ is given by

$$M(\xi) = \frac{(1-\xi^2)^2}{1 + 1.37\xi - 0.37\xi^4}. \tag{1.6}$$

The expressions in Eqs. (1.4) and (1.5) are the main analytical results of this work.

The expression in Eq. (1.5) presents the diffusion resistance as a sum of the diffusion resistance of the cylindrical channel without a partition, Eq. (1.3), and an additional diffusion resistance due to the presence of the partition, denoted by $\delta R_{\rm dif}$,

$$R_{\rm dif} = R_{\rm dif}^{\rm cyl} + \delta R_{\rm dif}, \tag{1.7}$$

where

$$\delta R_{\rm dif} = \frac{1}{2bD} M(\xi). \tag{1.8}$$

When $b = a$ (cylindrical channel), $\xi = 1$ and $M(\xi) = 0$. As a consequence, $\delta R_{\rm dif} = 0$, and Eq. (1.4) reduces to the expression for the flux through the cylindrical channel without a partition, Eq. (1.2). As ξ increases from zero ($b = 0$) to unity ($b = a$), function $M(\xi)$ monotonically decreases from unity to zero. Thus, as the hole radius tends to zero, the additional diffusion resistance diverges, and its asymptotic behavior is given by $\delta R_{\rm dif} = 1/(2bD)$, $b \to 0$.

Motivation for this study comes from the recognition that practically all protein channels of biological membranes studied so far contain the so-called constrictions in their water-filled pores. Indeed, examination of the high-resolution crystal structures of biological ion channels demonstrates that the pore geometries are very different from those of regular cylinders. Even relatively large and, therefore, poorly ion-selective channels, which have beta-barrel scaffolds as their major structural motif, are no exemptions. For the beta barrel itself a cylinder is indeed a good approximation, but these channels have certain structural elements that reside inside the barrel and create constrictions. In the case of bacterial porins, these structural elements are formed by the loops connecting beta strands of the barrel, which fold back into the pore leading to a significant local reduction of the pore cross section [2,3]. Another important example, an archetypical beta-barrel channel VDAC—voltage dependent anion channel of the outer mitochondrial membrane—also has a profound constriction, which is formed by the N-terminal alpha helix of the VDAC molecule [4–6]. The helix, located approximately halfway through the VDAC water-filled pore, reduces the beta-barrel effective diameter of about 3.0 nm by the helix diameter of 1.2 nm.

The geometry with a constriction is also a common feature of the highly ion-selective channels of neurophysiology. These channels, with mostly alpha-helical structures, discriminate between different ions with the help of a selectivity filter represented by the narrowest part of the pore. The size of the filter aperture is close to that of a dehydrated ion, which is a prerequisite underlying the mechanism of their action [7,8]. However, consideration of ionic transport is beyond the scope of the present study as it must include, in addition to entropic interactions, important electrostatic interactions [9,10].

It is worth mentioning that the studies of the effect of the constriction on various transport processes have a long history. Theoretical analysis of this class of problems was initiated by Maxwell and Lord Rayleigh in the nineteenth century [11,12]. One of the results of the present work is a simple formula for the diffusion resistance of a channel with the constriction, modeled as an infinitely thin partition with a circular hole in its center, Eq. (1.8). The formula covers the entire range of the hole radius and is derived by reducing the initial three-dimensional diffusion problem to a one-dimensional one. This is achieved by replacing the reflecting partition with the hole by an effective uniformly permeable partition. To determine the permeability of the effective partition we take advantage of the result found earlier [13] for trapping of particles diffusing in a cylindrical tube terminated by a reflecting wall containing an absorbing disk in its center. This result was obtained with the method of boundary homogenization. The accuracy of the approximation based on the replacement of the partition with a hole by a uniform partition and the range of applicability of such a replacement were established by comparing the predictions of our analytical approach with the results of Brownian dynamics simulations.

The outline of this paper is as follows. The expressions for the flux and diffusion resistance, Eqs. (1.4) and (1.5), are derived in the following Sec. II. The range of their applicability is established in Sec. III. Then in Sec. IV we discuss the relation of the expression for the additional diffusion resistance, Eq. (1.8), with corresponding results derived in a different field by a completely different method. Some concluding remarks are made in the final Sec. V.

II. THEORY

To derive the expressions in Eqs. (1.4) and (1.5), we take advantage of an approximate one-dimensional description of the solute dynamics in the channel, which, as shown in Sec. III, is applicable when the channel is long enough. The point is that sufficiently far away from the partition, located in the middle of the channel, the solute is uniformly distributed over the channel cross section, and its concentration depends only on the coordinate x measured along the channel axis, $c(x)$. In this case, we can introduce the one-dimensional steady-state concentration $c_1(x)$, defined as

$$c_1(x) = \pi a^2 c(x), \tag{2.1}$$

which satisfies

$$-D\frac{dc_1(x)}{dx} = J. \tag{2.2}$$

Although the concentration near the partition is not uniformly distributed over the cross section, nevertheless, it is assumed that Eq. (2.2) is also applicable in this region. Solving this equation, we obtain

$$c_1(x) = \begin{cases} c_{1-}(x) = \pi a^2 c_L - \frac{J}{D}(x - x_L), & x_L \leqslant x < (x_L + x_R)/2 \\ c_{1+}(x) = \pi a^2 c_R + \frac{J}{D}(x_R - x), & (x_L + x_R)/2 < x \leqslant x_R \end{cases}, \tag{2.3}$$

where c_L and c_R are the solute concentrations in the left (L) and right (R) reservoirs, and x_L and x_R are the coordinates of the left and right boundaries of the channel.

The one-dimensional concentrations on the two sides of the partition are not equal. To find the concentration jump on the partition, we treat the partition with the hole as a homogeneous semipermeable one, characterized by the effective permeability P. This is a key step in the approximate reduction of the initial three-dimensional problem to the equivalent one-dimensional one. The concentration difference on the two sides of the partition and the flux J are related by the condition

$$J = P\{c_{1-}[(x_L + x_R)/2] - c_{1+}[(x_L + x_R)/2]\}, \tag{2.4}$$

where $c_{1\pm}((x_L + x_R)/2)$ are the solute concentrations on the $+$ and $-$ sides of the partition given by Eq. (2.3),

$$c_{1-}[(x_L + x_R)/2] = \pi a^2 c_L - \frac{J}{2D}L \tag{2.5}$$

and

$$c_{1+}[(x_L + x_R)/2] = \pi a^2 c_R + \frac{J}{2D}L. \tag{2.6}$$

We take that the partition permeability P is one half of the effective trapping rate κ of solute molecules diffusing in a cylinder of radius a and trapped by a circular absorbing disk of radius b located in the center of the otherwise reflecting wall normal to the cylinder axis, $P = \kappa/2$.

An approximate expression for κ is obtained in Ref. [13] by the method of boundary homogenization. This method exploits the fact that the steady-state concentration of solute molecules diffusing to the absorbing disk sufficiently far away from the wall containing this disk is uniform over the cylinder cross section. As a consequence, one cannot distinguish between the flux to the absorbing disk on the otherwise reflecting wall and the flux to a partially absorbing uniform wall with a properly chosen trapping rate κ. An approximate expression for κ obtained in Ref. [13] is

$$\kappa = \frac{4Db}{\pi a^2} f(\xi), \tag{2.7}$$

where $\xi = b/a$ and function $f(\xi)$ is given by

$$f(\xi) = \frac{1 + 1.37\xi - 0.37\xi^4}{(1 - \xi^2)^2}. \tag{2.8}$$

Function $M(\xi)$ defined in Eq. (1.6) is the inverse of function $f(\xi)$,

$$M(\xi) = \frac{1}{f(\xi)}. \tag{2.9}$$

Substituting $c_{1\pm}[(x_L + x_R)/2]$ given in Eqs. (2.5) and (2.6) into Eq. (2.4) and solving the resulting linear equation for the flux J, we find

$$J = \frac{\pi a^2 P}{1 + PL/D}\Delta c = \frac{\pi a^2 D}{L + 2D/\kappa}\Delta c. \tag{2.10}$$

Finally, using the expression for κ in Eq. (2.7), we recover the results in Eqs. (1.4) and (1.5). Application of the approach based on boundary homogenization is justifiable when the channel is long enough. We establish what "long enough channel" means, as well as the range of applicability of the obtained results, in the following Sec. III.

III. RANGE OF APPLICABILITY

In this section, we take advantage of three-dimensional Brownian dynamics simulations to find the range of applicability of the approximate one-dimensional description of the solute dynamics in the channel used in Sec. II to derive the results in Eqs. (1.4) and (1.5). In our simulations we compute the mean first-passage time of a solute molecule between the channel ends. In the presence of the partition this time is longer than its counterpart in the cylindrical channel without a partition. As we will see, the increase of the mean first-passage time is proportional to the diffusion resistance of the partition $\delta R_{\rm dif}$.

To find the mean first-passage time consider the same cylindrical channel of length L and radius a, but now terminated by reflecting and absorbing boundaries at $x_L = 0$ and $x_R = L$, respectively. The mean lifetime of a solute molecule starting from the left (reflecting) boundary, which is the mean first-passage time from the left to the right boundary, denoted by $\tau_{\rm cyl}$, is given by [14]

$$\tau_{\rm cyl} = \frac{L^2}{2D}. \tag{3.1}$$

In the presence of an infinitely thin partition with a hole this mean first-passage time increases and can be written as

$$\tau = \tau_{\rm cyl} + \delta\tau, \tag{3.2}$$

where $\delta\tau$ is the delay time. When (1) the partition is in the middle of the channel, (2) its hole, located in the center of the partition, is circular and has radius b, and (3) the channel is long enough, the delay time is given by

$$\delta\tau = \frac{L}{\kappa} = \frac{\pi a^2 L}{4bD}M(\xi). \tag{3.3}$$

This is derived at the end of this section using the same approach based on the method of boundary homogenization as in Sec. II.

According to Eqs. (3.3) and (1.8) the delay time is proportional to the additional diffusion resistance,

$$\delta\tau = \frac{\pi a^2 L}{2}\delta R_{\rm dif}. \tag{3.4}$$

We take advantage of this to establish the range of applicability of our approach by comparing the delay time $\delta\tau$ predicted by the theory, Eq. (3.3), with its counterpart $\delta\tau_{\rm sim}$ obtained from three-dimensional Brownian dynamics simulations. In the simulations we determine the mean first passage time of a diffusing point particle from the reflecting to the absorbing boundary, denoted by $\tau_{\rm sim}$, defined as

$$\tau_{\rm sim} = \frac{1}{N}\sum_{i=1}^{N} t_i, \tag{3.5}$$

where $N = 25\,000$ is the number of diffusing particles used in our simulations, whose starting points are uniformly distributed over the reflecting boundary, and t_i is the lifetime of the i th particle. We find $\delta\tau_{\rm sim}$ by subtracting from $\tau_{\rm sim}$ the mean particle lifetime $\tau_{\rm cyl}$ in the channel without a partition, Eq. (3.1),

$$\delta\tau_{\rm sim} = \tau_{\rm sim} - \tau_{\rm cyl}. \tag{3.6}$$

Then we use Eq. (3.3) to find $M(\xi)$. In our simulations the particle trajectory can freely cross the hole in the partition in both directions, while its crossing the reflecting part of the partition or the side wall of the cylinder is treated as an elastic collision. When running the simulations, we take $a = 1$, $D = 1$, and the time step $\Delta t = 10^{-6}$, so that $\sqrt{2D\Delta t} = \sqrt{2}\times 10^{-3} \ll b_{\rm min}$, where $b_{\rm min}$ is the minimum size of the hole, $b_{\rm min} = 0.1$.

The results for a relatively long channel, $L = 2a$, are shown in Fig. 2 by the open circles. One can see that the values of $M(\xi)$ inferred from the simulations agree well with those predicted by our approximate one-dimensional description, Eq. (1.6), shown by solid curve. The relative errors (in percent) in the theoretically predicted delay times, Eq. (3.3), are compared to their counterparts obtained from the Brownian dynamics simulations in Table I for channels of lengths $L/a = 0.25$, 0.5, 0.75, 1, 2, 3, 4, and 5, with partitions having holes of radii $b/a = 0.1$, 0.2, 0.3, 0.4, 0.5, and 0.6. One can see that for sufficiently long channels, $L \geqslant a$, the relative error is less than 4%. Thus, the theory based on the boundary homogenization holds when the channel length exceeds its radius. For shorter channels, the theory fails since the reduction to the one-dimensional description is no longer valid. The problem is essentially multidimensional in this case.

Concluding this section, we derive the expressions in Eqs. (3.1)–(3.3). To this end, consider a particle diffusing in a long cylindrical channel of length L and radius a terminated by reflecting and absorbing boundaries at $x = 0$ and $x = L$, respectively. In the middle of the channel there is an infinitely thin partition with a circular hole of radius $b < a$ in its center. To derive the expression for the mean lifetime of a particle starting from the reflecting boundary, we use the approximate one-dimensional description of the solute dynamics in the channel discussed in Sec. II. Let $G(x,t)$ be the propagator of

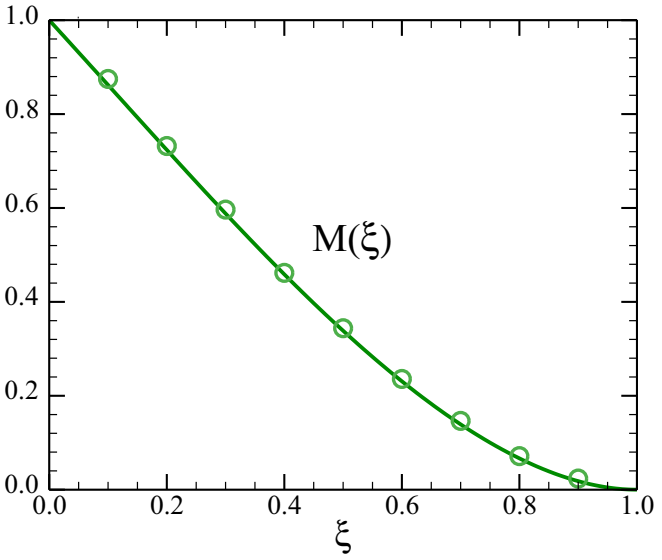

FIG. 2. Function $M(\xi)$, solid curve drawn according to Eq. (1.6), compared to $M(\xi)$ values, open circles, calculated using Eq. (3.3) with $\delta\tau$ obtained from Brownian dynamics simulations, $\delta\tau = \delta\tau_{\rm sim}$, for $D = 1$, $a = 1$, and $L = 2$.

a particle that starts from $x = 0$ at time $t = 0$. This propagator satisfies

$$\frac{\partial G(x,t)}{\partial t} = D\frac{\partial^2 G(x,t)}{\partial x^2}, \quad 0 < x < L/2, \quad L/2 < x < L, \tag{3.7}$$

subject to the reflecting and absorbing boundary conditions at the channel ends

$$\left.\frac{\partial G(x,t)}{\partial x}\right|_{x=0} = G(L,t) = 0, \tag{3.8}$$

and the matching conditions at $x = L/2$,

$$\left.\frac{\partial G(x,t)}{\partial x}\right|_{x=\frac{L}{2}-0} = \left.\frac{\partial G(x,t)}{\partial x}\right|_{x=\frac{L}{2}+0} = -\frac{\kappa}{2D}\left(G|_{x=\frac{L}{2}-0} - G|_{x=\frac{L}{2}+0}\right), \tag{3.9}$$

TABLE I. The relative errors (in percent) in the theoretically predicted delay times, Eq. (3.3), compared to their counterparts obtained from the Brownian dynamics simulations.

	L/a							
b/a	0.25	0.50	0.75	1.0	2.0	3.0	4.0	5.0
0.10	10.34	2.88	2.53	1.97	1.43	1.56	1.19	1.24
0.20	16.02	2.17	1.57	0.32	1.04	1.39	0.97	1.04
0.30	20.98	3.43	1.76	1.62	1.25	2.41	0.66	0.17
0.40	21.46	3.97	3.48	1.53	0.43	3.40	0.81	1.37
0.50	21.10	4.92	1.88	2.39	1.15	3.62	2.58	1.61
0.60	18.47	5.21	1.92	3.07	1.33	3.43	0.71	3.61

as well as the initial condition $G(x,0)=\delta(x)$. In Eq. (3.9) we have taken into account the fact that the permeability of the effective uniform partition is one half of the trapping rate κ.

The particle survival probability for time t, denoted by $S(t)$, is the integral of the propagator over the particle position x in the channel,

$$S(t)=\int_0^L G(x,t)\,dx. \tag{3.10}$$

The probability density of the particle lifetime in the channel, $\varphi(t)$, is

$$\varphi(t)=-\frac{dS(t)}{dt}. \tag{3.11}$$

Using this, one can check that the mean particle lifetime is the integral of its survival probability over time from zero to infinity,

$$\tau=\int_0^\infty t\varphi(t)dt=\int_0^\infty S(t)\,dt. \tag{3.12}$$

Substituting here $S(t)$ in Eq. (3.10) and changing the order of integration, we arrive at

$$\tau=\int_0^L \rho(x)\,dx, \tag{3.13}$$

where function $\rho(x)$ is the density of the mean residence time spent by the particle at point x,

$$\rho(x)=\int_0^\infty G(x,t)\,dt. \tag{3.14}$$

Integrating Eqs. (3.7)–(3.9) over time from zero to infinity, one finds that the function $\rho(x)$ satisfies

$$D\frac{d^2\rho(x)}{dx^2}=-\delta(x),\quad 0<x<L/2,\quad L/2<x<L, \tag{3.15}$$

subject to the reflecting and absorbing boundary conditions at the channel ends

$$\left.\frac{d\rho(x)}{dx}\right|_{x=0}=\rho(L)=0, \tag{3.16}$$

and the matching condition at $x=L/2$,

$$\left.\frac{d\rho(x)}{dx}\right|_{x=\frac{L}{2}-0}=\left.\frac{d\rho(x)}{dx}\right|_{x=\frac{L}{2}+0}=-\frac{\kappa}{2D}\left[\rho\left(\frac{L}{2}-0\right)-\rho\left(\frac{L}{2}+0\right)\right]. \tag{3.17}$$

Solving the above equation, we obtain

$$\rho(x)=\frac{1}{D}(L-x)+\frac{2}{\kappa}H\left(\frac{L}{2}-x\right), \tag{3.18}$$

where $H(z)$ is the Heaviside step function, $H(z)=0$ when $z<0$, and $H(z)=1$ when $z>0$. Substituting $\rho(x)$ into Eq. (3.13) and performing the integration, we arrive at Eq. (3.2) with $\tau_{\rm cyl}$ and $\delta\tau$ given by Eqs. (3.1) and (3.3), respectively.

IV. DISCUSSION

In 1941, V. A. Fock, who is well known to the chemical physics community for his work in atomic physics (Hartree-Fock method), considered the effect of infinitely thin partition with a circular hole in its center on the steady flow of electric current down a long circular tube filled with a conducting medium [15]. Fock calculated the additional electrical resistance δR_{el} due to the presence of the partition. His result in our notations can be written as

$$\delta R_{el}=\frac{1}{2b\sigma}M_{\rm Fock}(\xi), \tag{4.1}$$

where σ is the conductivity of the medium, $\xi=b/a$, a and b are the tube and hole radii, respectively, and $M_{\rm Fock}(\xi)$ is the Fock result for the function $M(\xi)$ defined in Eqs. (1.6) and (2.9). Comparison of the above expression for δR_{el} and the expression for the additional diffusion resistance $\delta R_{\rm dif}$, Eq. (1.8), shows that the two additional resistances have the same algebraic form. This is a consequence of the fact that the densities of both the diffusion flux and electric current are gradients of scalar fields (concentration and electric potential, respectively), which satisfy the same Laplace equation, and both satisfy reflecting boundary conditions on the walls.

Fock obtained an approximate solution for the function $M_{\rm Fock}(\xi)$ in the form of a power series expansion in ξ,

$$M_{\rm Fock}(\xi)=1+\sum_{n=1}^{\infty}a_n\xi^n. \tag{4.2}$$

He evaluated coefficients a_n in terms of the integrals of the Bessel functions and gave numerical values of the first 12 coefficients a_n. Fock also proposed a simple truncated expression for $M_{\rm Fock}(\xi)$,

$$M_{\rm Fock}(\xi)=1-1.41\xi+0.34\xi^3+0.07\xi^5, \tag{4.3}$$

which gives correct values of $M_{\rm Fock}(\xi)$ at $\xi=0$ and $\xi=1$, $M_{\rm Fock}(0)=1$, and $M_{\rm Fock}(1)=0$. The series in Eq. (4.2) converges rapidly, as $\xi\to 0$, and very slowly, as $\xi\to 1$. The exact asymptotic behavior of function $M(\xi)$ in the second limiting case was obtained by Leppington and Levine [therefore, here and in Eq. (4.4) the subscript *Fock* in the function $M_{\rm Fock}(\xi)$ is omitted], who showed that [16]

$$M(\xi)=2(1-\xi)^2,\quad \xi\to 1. \tag{4.4}$$

It is instructive to compare the above-mentioned results with the expression for function $M(\xi)$, Eq. (1.6), obtained using the method of boundary homogenization. As follows from Eq. (1.6) the asymptotic behavior of $M(\xi)$ is given by

$$M(\xi)=\begin{cases}1-1.37\xi, & \xi\to 0\\ 2(1-\xi)^2, & \xi\to 1\end{cases}. \tag{4.5}$$

Comparison of this asymptotic behavior with those predicted by Eqs. (4.3) and (4.4) for $\xi\to 0$ and $\xi\to 1$, respectively, shows that boundary homogenization provides quite accurate solution for function $M(\xi)$ in both limiting cases. Comparing the plots of functions $M(\xi)$ and $M_{\rm Fock}(\xi)$, given in Eqs. (4.3) and (1.6), respectively, one can check that they are indistinguishable by eye over the entire range of ξ.

V. CONCLUDING REMARKS

The main results of this work are Eqs. (1.4) and (1.5). The former gives the steady-state flux of solute molecules through a cylindrical membrane channel with an infinitely thin partition located in the middle of the channel, which has a circular hole in its center. The latter is the diffusion resistance of such a channel, which is the sum of the diffusion resistance of the cylindrical channel without a partition and the additional diffusion resistance due to the presence of the partition, Eqs. (1.7), (1.3), and (1.8). These expressions have been derived using an approximate one-dimensional description of solute dynamics in the channel. In this approach the nonuniform partition with a hole is treated as a uniform semipermeable partition. To find its effective permeability P we have taken advantage of the result obtained earlier [13] for trapping of solute molecules diffusing in a cylindrical tube terminated by a reflecting wall perpendicular to the tube axis containing an absorbing disk in its center. Using the method of boundary homogenization, in Ref. [13] it was shown that trapping by an inhomogeneous terminating wall can be approximately described as that by a homogeneous partially absorbing wall with properly chosen trapping rate κ. We have assumed that the effective permeability is one half of this trapping rate. Having in hand κ, given by Eq. (2.7), we can find the permeability, $P = \kappa/2$.

The same approach based on boundary homogenization can also be applied in the case of a partition containing a large number, $N \gg 1$, of small holes of radius $b \ll a$. The two cases differ only in the expressions for the effective trapping rate κ. In the case of $N \gg 1$ this trapping rate, denoted by κ_N, is given by

$$\kappa_N = \frac{4Db}{\pi a^2} N f_N(\sigma), \tag{5.1}$$

where $\sigma = Nb^2/a^2 = N\xi^2$ is the surface fraction of the partition occupied by holes and function $f_N(\sigma)$ is

$$f_N(\sigma) = \frac{1 + A\sqrt{\sigma} - B\sigma^2}{(1-\sigma)^2}. \tag{5.2}$$

The coefficients A and B depend on the arrangement of the holes on the partition. One can find the values of these coefficients for the triangular, square, and hexagonal lattices of the holes, as well as for their random uniform distributions over the partition in Ref. [13].

When the hole in the partition is small compared to the channel radius, our results can be generalized to the case of noncircular holes. This can be achieved by replacing in the above formulas the hole radius b by an effective radius $b_{\rm eff}$, which is a function of the area S and perimeter P of the hole,

$$b_{\rm eff} = \left(\frac{SP}{2\pi^2}\right)^{1/3}. \tag{5.3}$$

As shown in Ref. [17], trapping of diffusing particles by a noncircular absorbing spot on the otherwise reflecting flat wall to a good approximation is the same as that by a circular disk whose radius is related to the spot area and perimeter by Eq. (5.3). This is true on condition that the spot is only moderately asymmetric, and its boundaries are not too jagged.

Our analysis of transport through a channel with a partition utilizes known results for the effective trapping rate κ by inhomogeneous surfaces, Eqs. (2.7) and (5.2). These results were obtained in the theory of diffusion-limited reactions by the method of boundary homogenization, which allows one to get relatively simple formulas for the effective trapping rate by inhomogeneous surfaces in highly nontrivial geometries [13,18–24]. Here we have demonstrated how some of these formulas can be used beyond the scope of diffusion-limited kinetics. We believe that there are problems in different areas of science and engineering where the results found with the method of boundary homogenization may help to derive approximate solutions that cannot be obtained by other methods.

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