Exact Solution for a Spherical Source and Internally Reactive Sink

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This paper presents the rigorous solution for the diffusive interaction between a reactant source and a sink with a volume distributed internal consumption reaction. While in applications sinks are often impenetrable with surface consumption reactions[1,2], a number of important cases of penetrable sinks with internal reactions can be found. In the analysis of interacting mixed microbial populations, sometimes two different cellular species exchange growth factors for a common form of *mutualism*.[3] Still more widespread are commensal relationships, where one species produces a compound (a vitamin, growth factor or nutrient), which causes the growth of another species (See page 640 of reference 3 for a list of examples.)

The two cell problem can be solved with bispherical expansion[4,5] or bispherical coordinates[6]. Here the twin spherical expansion is used and each cell has a spherical coordinate originating at the center where the radial component is $r_{1(2)}$ and angle $\Omega_{1(2)}$ is positive in the counterclockwise direction (Figure 1). Any point in the system can be expressed in either set of spherical coordinates.

The spherical source can have any radius a_2, and in reference 1 it is shown that a steady, uniform rate σ of reactant delivery per unit external surface area is appropriate for the mutualism and commensal interaction[1,3,7]. The source cell must take up as substrates the needed precursor chemicals for the mutualism or commensal reactant compound; carry out intracellular processes to break down the input, manufacture the reactant and expel the reactant from the source cell wall. A very common experimental substrate uptake rate for a cell is Monod-type kinetics. If we assume reasonable reactant precursor substrate concentrations Monod kinetics suggest a zeroth order uptake kinetics, because the denominator constant is usually small.[3] A pseudo-steady state cell implies a zeroth order chemical production of reactant from the source cell surface.[7] The extracellular reactant transport outside the source and sink volumes is by Fickian diffusion with diffusivity D and reactant concentration c. The spherical sink may have an arbitrary radius a_1, and is located a center-to-center distance d from the spherical source cell (Figure 1). The concentration of the mutualism or commensal reactant vitamin or growth factor is often low, so that the volumetric reaction rates within the sink can be considered to be first order with a reaction rate constant k_{int}. The reactant transport within the sink is modeled as Fickian with an effective internal diffusion coefficient D_{int}[8]. The Fundamental geometrical, kinetic and transport parameters can be combined into three dimensionless groups

$$\gamma = a_1 / a_2 , \tag{1}$$

$$d_1 = d / a_1 , \tag{2}$$

$$\varepsilon = D / D_{\text{int}} , \tag{3}$$

and an internal sink Thiele modulus[9]

$$\phi_T = a_1 \sqrt{k_{\text{int}} / D_{\text{int}}} . \tag{4}$$

The net dimensionless volume distributed sink reaction rate expression

$$P = \left(4\pi a_2{}^2 \sigma\right)^{-1} a_1^2 D \int \mathbf{n_1} \bullet \nabla c \; d\Omega_1 , \tag{5}$$

depends on the values of the four dimensionless quantities (1) – (4) given above. The integral in equation (5) is over the sink surface and contains all elements of solid angle $d\Omega_1$, $\boldsymbol{\eta}_1$ is the sink surface unit normal vector within $d\Omega_1$ pointing away from the sink surface into the extracellular space. In yet another application, the quantity P is the probability that a molecule emitted from a zeroth order source surface diffuses to the sink and is trapped within the internal volume, is the well known steady-state trapping problem in the chemical physics literature[10,11,12].

In an earlier paper[1] rigorous, exact expressions were derived both for the sink reaction rate P and the local reactant concentration c for the same zeroth order spherical source, but for a first order surface reaction with rate constant k_{s1} or an impenetrable sink. While the dimensionless quantities γ and d_1 remain the same, only a single dimensionless sink surface reaction rate constant k_1

$$\lambda^{-1} = k_{s1}a_1 / D, \tag{6}$$

is needed to completely characterize the impenetrable sink reactivity P. The P and c results were presented in reference 1 as exact solutions for the impenetrable sink applications, but they are also useful as an approximation for the penetrable sink cases. In this communication, the conditions under which the use of an effective surface reactivity k_{1eff} and the impenetrable sink results of reference 1 will accurately describe the volume reaction P for a penetrable sink, and when it will fail will be examined.

The solution of the source-penetrable sink can be generated directly from the source-impenetrable sink forms[1]. From reference 1, the λ dependence of the impenetrable sink P and c can be entirely included in coefficients Λ_n of the form

$$\Lambda_n = (1 - n\lambda)/[1 + (n+1)\lambda], \qquad n = 0,1,2,..... \tag{7}$$

Tsao[13], in the context of the physically different problem of two identical sink in the presence of a uniform, constant reactant concentration, has shown that the impenetrable sink solutions will produce the corresponding penetrable sink quantities upon the substitution of Θ_n for Λ_n,

$$\Lambda_n \to \Theta_n = (1 - n\lambda_n)/[1 + (n+1)\lambda_n], \tag{8}$$

$$\lambda_n = D i_n(\phi_T) / D_{\text{int}} \phi_T i_n^{'}(\phi_T), \tag{9}$$

where i_n is related to the modified Bessel function of half-integer order $I_{n+1/2}(\phi_T)$ by

$$i_n(\phi_T) = \sqrt{\pi / 2\phi_T}\, I_{n+1/2}(\phi_T), \tag{10a}$$

and i_n' is the first derivative[14]

$$i_n^{'}(\phi_T) = \frac{d}{dx}\left(i_n(x)\right)\Big|_{x=\phi_T} = i_{n-1}(\phi_T) - \frac{n+1}{\phi_T} i_n(\phi_T), \tag{10b}$$

and in general $\Lambda_n \neq \Theta_n$. The substitution (8) comes directly from comparing the sink surface boundary conditions for an impenetrable and penetrable sink and the same relationship can be shown to be valid for the source-sink problem. As the details of the source-penetrable sink derivations are similar to those in reference 1, they are omitted and the final results for the trapping probability are listed below. Applying the substitution (8) – (9) directly into the P expression, equations (20), (24), (25) and (31) of reference 1, we have

$$P = d_1^{-1}\Theta_0\left[1+\sum_{n=0}^{\infty} Q_n^{(n)} K_{0n}^{(n)}\left(1-K_{nn}^{(n)}\right)^{-1}\right], \qquad (11)$$

for the closed fraction type forms

$$K_{nm}^{(i+1)} = K_{nm}^{(i)} + K_{im}^{(i)} K_{ni}^{(i)}\left(1-K_{ii}^{(i)}\right)^{-1}, \qquad (12)$$

$$K_{nm}^{(0)} = -d_1^{-(2m+2)}\gamma^{-1}\Theta_m I_{nm}\left(d_1^{-2}\gamma^{-2}\right), \qquad (13)$$

with

$$I_{00}(x) = (1-x)^{-1} + \frac{1}{x}\ln(1-x), \quad \text{for } x = (\gamma d_1)^{-2} \qquad (14a)$$

and

$$I_{n0}(x) = (1-x)^{-(n+1)} - (nx)^{-1}\left[(1-x)^{-n} - 1\right] \quad \text{for } n \neq 0, \qquad (14b)$$

$$I_{nm}(x) = \frac{x}{m!}\frac{d}{dx}\left\{\frac{1}{x}\frac{d^{m-1}}{dx^{m-1}}\left[x^m (1-x)^{-(n+1)}\right]\right\} \quad \text{for } n \neq 0, \ \ m \neq 0, \qquad (14c)$$

and

$$Q_n^{(i+1)} = Q_n^{(i)} + Q_i^{(i)} K_{ni}^{(i)}\left(1-K_{ii}^{(i)}\right)^{-1}, \qquad (15)$$

with

$$Q_n^{(0)} = 1. \qquad (16)$$

The solution form (11) – (16) contains only one summation (11), and each term of P needs only a finite number of n nested steps for its exact evaluation, and P is guaranteed to converge for any set of parameters (1) – (4).

Now the question is posed, is there some selection of an effective surface reaction rate k_{1eff}, written in terms of ε and ϕ_T, that when used in λ within the solution of reference 1, will give the same P behavior as equations (11) – (16)? One reasonable choice of k_{1eff} is to match the overall sink reaction rates of the impenetrable and penetrable isolated sinks, because at least at infinite separation $d_1 \to \infty$ the results would always coincide, hence we select

$$k_{1eff} = \left(D_{\text{int}}/a_1\right)\left(\phi_T \coth \phi_T - 1\right). \qquad (17)$$

For the different problem of pure competition between two identical sinks, Tsao[13] has stated that the impenetrable sink solutions written in terms of Λ_0 can be used with good accuracy to model the penetrable sink results upon the substitution of Θ_0 for Λ_0. Tsao's[13] procedure is the same as the use of equation (17) into λ suggested above. One advantage of this substitution is that the penetrable sink problem is reduced from a four parameter problem to a three parameter problem with

$$\lambda_{1eff}^{-1} = k_{1eff}\, a_1/D \qquad (18)$$

replacing the ε and ϕ_T. A second advantage is all the chemical physics phenomena found for the source impenetrable sink problem[1] apply directly to the penetrable sink case.

It turns out that the impenetrable sink solutions of reference 1 with an effective inverse surface reaction rate coefficient λ_{1eff} of equation (17) and (18) reproduce the penetrable sink behavior of equations (11) – (16) rather well, except in one region of the total parameter space, $\phi_T < 0.5$ and $\varepsilon < 0.5$. Typical behavior is shown in Figure 2 where the trapping probability is plotted versus the dimensionless separation distance $d/(a_1 + a_2)$ for equisized spheres $\gamma = 1$, a Thiele modulus of $\phi_T = 0.01$ and a diffusivity ratio $\varepsilon = 0.1$. The solid line represents P values from equations (11) – (16) and the dotted line, which lies above it, is the source impenetrable sink solution from reference 1 using λ_{1eff} from equations (17) and (18). As expected the two solutions approach each other as the dimensionless distance d_1 increases, but as true contact is approached the impenetrable approximation is in error by as much as -7.4%. Table 1, lists the error at contact for same sized spheres (γ=1) for values of the Thiele modulus $\phi_T < 0.5$ and for diffusivity ratios $\varepsilon < 0.5$. The observed discrepancies can be particularly significant, because as Weisz[15] points out nature evolves its microorganisms to use its internal space efficiently, cellular values of ϕ_T at or below 0.5 are not uncommon. It is likely that the same limitations should also be placed on Tsao's results[13], i.e. in the parameter region of Table 1 the full penetrable sink solutions should be used.

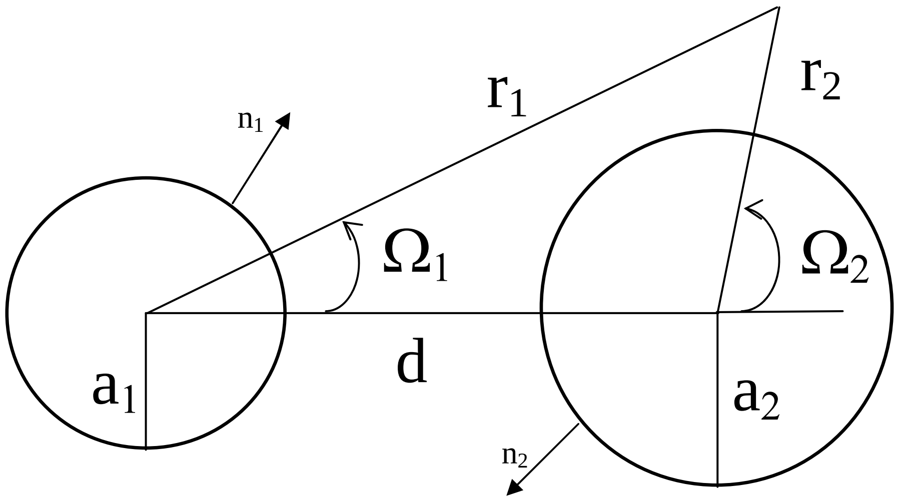

FIG. 1: Two spheres of radius a_1 and a_2, spherical coordinates (r_1, Ω_1 and r_2, Ω_2) separated by center-to-center distance d. Sphere 1 is the sink and sphere 2 is the source cell.

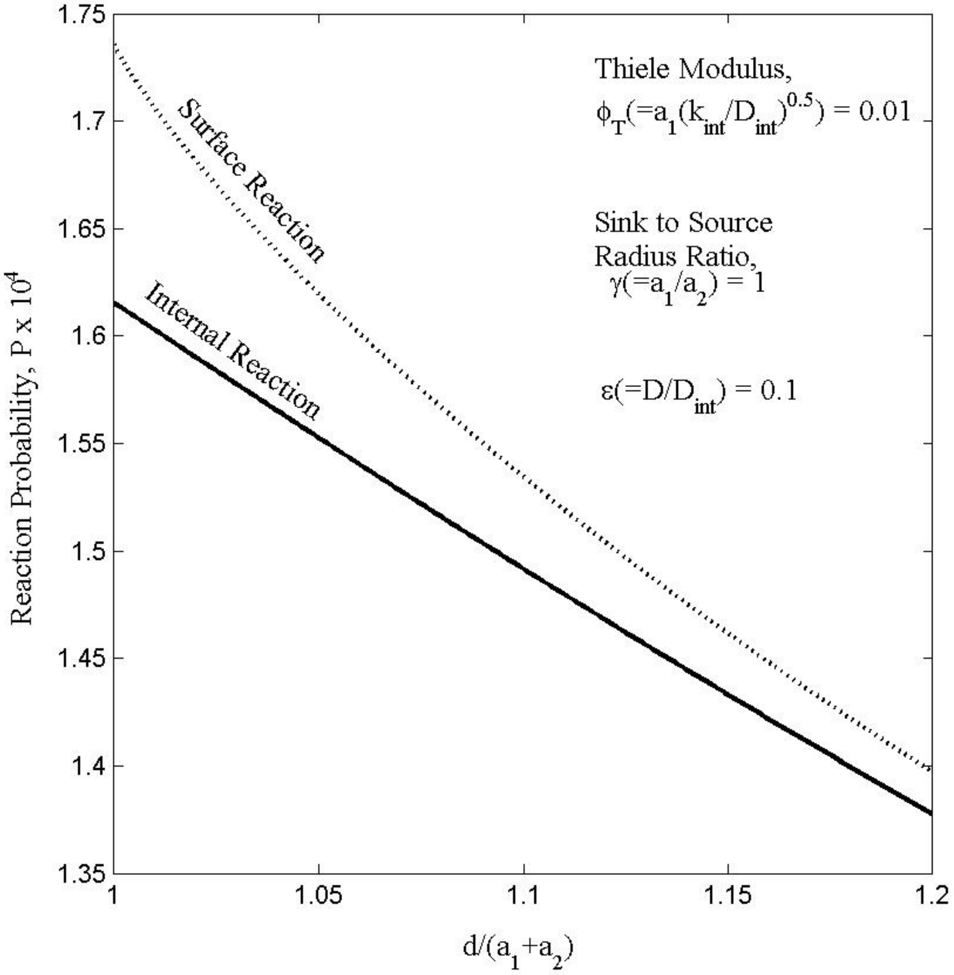

Figure 2: Reaction probability P versus the dimensionless center to center distance $d(a_1+a_2)^{-1}$ between the source and sink, for a sink to source radius ratio $\gamma(=a_1/a_2)$ of 1.0, extracellular to internal sink diffusivity ratio $\varepsilon(=D/D_{\text{int}})$ of 0.1 and sink Thiele Modulus $\phi_T(=a_1\sqrt{k_{\text{int}}/D_{\text{int}}})$ of 0.01. The lower solid line is the exact reaction probability from equation (11), for an internally reactive sink, and the dashed line refers to the approximate, sink surface reaction probability, from reference 1 with an effective inverse dimensionless reaction rate coefficient $\lambda_{1eff}^{-1}(=\varepsilon/(\phi_T \coth\ \phi_T - 1))$ of 3000.

PERCENT ERROR FOR THE EXACT AND APPROXIMATE SOLUTION

Table 1

ϕ_T	$\varepsilon = 0.5$	$\varepsilon = 0.1$	$\varepsilon = 0.05$	$\varepsilon = 0.01$
0.5	-4.48	-3.98	-2.94	-0.92
0.3	-5.06	-5.69	-4.92	-2.16
0.1	-5.39	-7.19	-7.35	-6.22
0.05	-5.43	-7.38	-7.71	-7.59
0.01	-5.43	-7.44	-7.83	-8.16

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