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Topological derivation of nonlinear convection-diffusion equations using network theory

Leonardo Peusner
P.O. Box 380, York, Maine 03909
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Convection-diffusion equations and equations for concentration profiles are derived using a simple network-theory technique which shows the bifurcation of the solutions when $J_v = 0$.

I. INTRODUCTION

Magenold and Solf[1] derived an equation that gives the coupling between solute and volume flows in a slab or membrane. By starting with the (apparently) linear local equation

$$J_s = c_{(x)}(1-\sigma)J_v + P_{(x)}\frac{\partial c}{\partial x} , \tag{1}$$

in which $P_{(x)}$ is the local permeability and σ the local reflection coefficient, a nonlinear global solution of the form

$$J_s = \left[\frac{c_0}{1-e^{-\lambda J_v}} + \frac{c_L}{1-e^{\lambda J_v}}\right] hJ_v \tag{2}$$

is obtained. This expression gives the steady-state flow of solute, J_s for a membrane of thickness L kept between concentrations $c_{(0)}$ and $c_{(L)}$. The parameters h and λ in Eq. (2) are given by

$$h = (1-\sigma)/\omega RT$$

and

$$\lambda = hL/P(x) .$$

This equation has been used many times, including in Teorell's analysis of his own membrane oscillator.[2] Mikulecky[3] points out that this equation is periodically rediscovered, and reviews close to a dozen references of cases in which it has appeared in different contexts. He also shows that the point $J_v = 0$ is a bifurcation point, and that it is smeared out by Kedem-Katchalsky's linearization,[4] thus leading to discrepancies in terms of reciprocity assumptions. Moreover, he also gives an equation for the concentration profiles,

$$\frac{c_{(0)} - c_{(x)}}{c_{(0)} - c_{(L)}} = \frac{1-e^{\lambda J_v x}}{1-e^{\lambda J_v}} , \tag{3}$$

in which x is normalized in terms of a unitless quantity and the total length of the membrane is 1.

The purpose here is to derive proper global equations using the (linear) methods of network theory and simple series one ports.[5-9] We shall show that (1) this method exposes the bifurcation at $J_v = 0$ and (2) Eq. (2) actually consists of *two* separate equations, one for $J_v > 0$, one for $J_v < 0$.

II. DISCRETE REPRESENTATION OF THE CONVECTION-DIFFUSION PROBLEM

We begin the analysis by subdividing the slab or membrane into N segments so that the local equations can be represented by the difference equations

$$J_s = c_i hJ_v + (c_i - c_{i_+})P_A , \tag{4}$$

in which $h = (1-\sigma)$, P_A is the local permeability of the subregion, and we have assumed the volume flow originates at i and moves toward i_+ (the plus-x direction). Equation (4) cannot be represented by a simple linear one-port resistor as it stands because—although it can be geometrically represented by a line—*it is not* a linear operator. The reason for this apparent paradox is that the presence of the constant term J_v introduces either a positive or negative bias at i—depending on the direction of J_v—which is modulated by the local concentration at i, but not related to $c_{i_{(+)}}$. However, Eq. (4) may be rearranged to yield the expression

$$J_s = P_A(1 + hJ_v/P_A)[c_i - c_{i_+}/(1 + hJ_v/P_A)] . \tag{5}$$

Equation (5) can now be modeled by a linear one-port resistance of value

$$R_d = \left[\frac{1}{1 + hJ_v/P_A}\right]\frac{1}{P_A} \tag{6}$$

placed between potentials of values c_i and $c_{i_+}/(1 + hJ_v/P_A)$, as indicated in Fig. 1. Note that the values of the resistance and the potentials vary both with position and J_v and that, moreover, the potentials are not simple concentrations, but modulated quantities.

This process may be continued on the whole slab by taking small resistive segments and matching the potential at the end of one resistance with the next, thus ensuring continuity of the process and allowing a single flow J_s to pass through all resistances in the steady state. We obtain, in the steady state, a string of resistances given by the series,

$$R_d^{(i)} = [P_A(1 + hJ_V/P_A)^i]^{-1} , \tag{7}$$

while the concentration fits the series described by the typical term

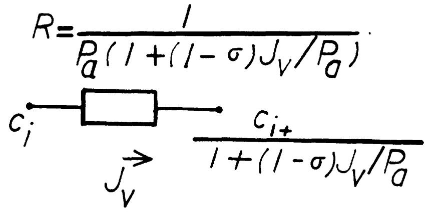

FIG. 1. Basic unit slab representing the convection-diffusion equation when the bulk flow J_v goes from left to right. The system may be represented by a linear resistance with convective-diffusional flow J_s going through and end potentials given by convection-modulated functions of the concentration. Notice that when $J_v=0$, the resistance simply reduces to an inverse permeability, R $(=1/P)$, while the potential difference across the resistance is simply given by the difference in concentration at the end points of the slab.

$$c_0, \ldots, [c_i/(1+hJ_v/P_A)^i], \ldots, [c_N/(1+hJ_v/P_A)^N] , \tag{8}$$

as shown in Fig. 2. The total convection-diffusion resistance may be found by adding individual series components. If we define the term

$$\frac{1}{F} \equiv \frac{1}{1+hJ_v/P_A} ,$$

the total resistance becomes

$$R_d^{\text{total}}=(1/P_A)\left[\frac{1}{F}+\frac{1}{F^2}+\cdots+\frac{1}{F^N}\right] , \tag{9}$$

a geometric progression which reduces to

$$R_d^{\text{total}}=\frac{1}{hJ_v}\left[1-\frac{1}{(1+hJ_v/P_A)^N}\right] . \tag{10}$$

The potential difference (force, X) between the end points is given, according to (8), by

$$X=[c_0-c_N/(1+hJ_v/P_A)^N] , \tag{11}$$

so that the resultant steady convection-diffusion flow is

$$J_s^{\rightarrow}=\frac{X}{R_d^{\text{total}}}=(c_0F^N-c_N)hJ_v/(F^N-1) , \tag{12}$$

in which $F=(1+hJ_v/P_A)$.

In the case in which the convective flow goes from right to left, the potentials must be redefined, starting from the right-hand side. The overall force X across the slab is then given by

$$X'=[c_0/(1+hJ_v/P_A)^N]-c_N$$
$$=(c_0/F^N)-c_N ,$$

while the total resistance still has the value (10). It then follows that the convection-diffusion flow is

$$J_s^{\leftarrow}=\frac{X^i}{R_d}=\frac{c_0-F^Nc_N}{(1/hJ_v)(F^N-1)} . \tag{13}$$

Note that Eqs. (12) and (13) represent two distinct solutions, thus showing the bifurcation at $J_v=0$. This bifurcation disappears in the limit of the Magenold and Solf approximation considered next.

III. LIMIT OF DOMINANT DIFFUSION RANGE MAGENOLD AND SOLF EQUATIONS

We can introduce the approximations

$$(1+x)^N \simeq 1+Nx+N(N-1)(x^2/2!)$$
$$+N(N-1)(N-2)(x^3/3!)+\cdots$$

for $(x \ll 1)$ and

$$e^{Nx} \simeq 1+Nx+N^2x^2/2!+N^3x^3/3!$$
$$+\cdots .$$

For large N and small x it follows that

$$e^{Nx} \simeq (1+x)^N ,$$

so that in the approximation $J_v/P_A \ll 1$, when diffusion is dominant,

$$(1+hJ_v/P_A)^N \simeq e^{hJ_vN/P_A} . \tag{14}$$

By introducing the normalization condition[3] $P_{(x)}/P_A=L/N$, Eq. (10) then simplifies to

$$R_d^{\text{total}}=\frac{1-e^{-\lambda J_v}}{hJ_v} , \tag{15}$$

while the force X is given by

$$X=c_0-c_Le^{-\lambda J_v} ,$$

in which c_L is the concentration at $x=L$ (the right-hand side of the slab). It then follows that the steady flow is given by

$$J_s=\frac{(c_0-c_Le^{-\lambda J_v})hJ_v}{(1-e^{-\lambda J_v})} ,$$

and further rearrangement leads to the expression

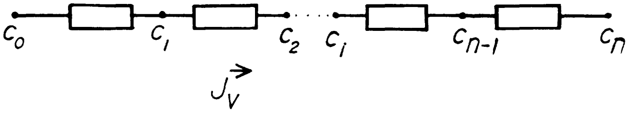

FIG. 2. The complete, global solution when several unit slabs are connected together is found by matching end potentials at neighboring slabs and changing the values of the resistances accordingly. Any element in the concentration series is given by $\phi_i=c_i/(1+hJ_v/P_A)$, in which ϕ_i is the potential at the given node. Note this potential equals the concentration at that point when the convective flow vanishes. The resistance between any two potentials is given by $R_i=[P_A(1+hJ_v/P_A)^i]^{-1}$.

$$J_s=\left[\frac{c_0}{1-e^{-\lambda J_v}}+\frac{c_L}{1-e^{\lambda J_v}}\right]hJ_v \; . \tag{16}$$

When the volume flow is in the negative direction, the potential difference becomes

$$[c_0/(1-hJ_v/P_A)^N]-c_N=c_0e^{\lambda J_v}-c_L \; , \tag{17}$$

while the resistance is still given by (10), with negative J_v:

$$R_d^{\text{total}}=\frac{1-e^{\lambda J_v}}{(-hJ_v)} \; . \tag{18}$$

The convection-diffusion flow for negative J_v is

$$J_s=\frac{X}{R_d}=\frac{c_0e^{\lambda J_v}-c_L}{1-e^{\lambda J_v}}(-hJ_v) \; ,$$

which leads, after further rearrangement, to

$$J_s=\left[\frac{c_0}{1-e^{-\lambda J_v}}+\frac{c_L}{1-e^{\lambda J_v}}\right]hJ_v \; . \tag{19}$$

While Eqs. (16) and (19) give the same analytical expression for positive and negative J_v, the network derivation shows, however, that they arise from different sets of global equations having different boundary conditions (potential differences). The two solutions are, in fact, distinct and correspond to the bifurcations for $J_v<0$ and $J_v>0$, as mentioned by Mikulecky.[3]

IV. CONCENTRATION PROFILES

The network can also be utilized to find the distribution of concentration profiles. If we wish to find the concentration at a point x (i in the network) relative to the left-hand-side concentration c_0, for example, we first note that node potentials are not concentrations, but are given instead by

$$\phi_i=\frac{c_i}{(1+hJ_v/P_A)^i}=c_ie^{-\lambda J_v x} \; .$$

To find the potential at any point we use the voltage divider relation

$$\frac{\phi_0-\phi_i}{\phi_0-\phi_n}=R_i/R_{\text{total}}=\frac{(1-e^{-\lambda J_v x})}{(1-e^{-\lambda J_v})} \; .$$

This leads to

$$(c_0-c_{(x)}e^{-\lambda J_v x})=(c_0-c_Le^{-\lambda J_v})\frac{(1-e^{-\lambda J_v x})}{(1-e^{-\lambda J_v})} \; .$$

Rearranging and solving for $c_{(x)}$ this expression can be written as

$$c_{(x)}=c_0e^{\lambda J_v x}-\frac{(e^{\lambda J_v x}-1)}{(e^{\lambda J_v}-1)}(c_0e^{\lambda J_v}-c_L) \; .$$

Further rearrangement leads to

$$c_{(x)}=c_0-(c_0-c_L)\frac{(1-e^{\lambda J_v x})}{(1-e^{\lambda J_v})}$$

in agreement with previous results [Eq. (3)].

V. DISCUSSION

From the above analysis, it is clear that the network approach is consistent with analytical results and, in addition, it brings out topological information which is buried or smeared in the analytical treatment.

Note that a key step in solving the convection-diffusion equations was to match the potentials and flows at neighboring regions, thus establishing a unique potential function at each point. Also, we should point out that the results obtained are consistent with the simple diffusion problem when $J_v=0$; in that limit the potentials become concentrations and the resistances reduce to diffusion resistances—i.e., Fick's law. The presence of the biasing flow J_v, on the other hand, distorts the linearity of diffusional space and changes the linear problem into a nonlinear problem. These properties of the diffusion-convection interaction would be completely buried if we attempted to analyze it by linearization techniques.

Clearly, numerical results could be obtained easily from the network representations (12) and (13). The error involved in the discretization is treated in standard texts.[10]

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