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Distribution of a Trace Element in a Boundary Layer with Mass Transfer

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A theory is presented for the downstream distribution of a tracer injected into a boundary layer of a flat plate or cone with self-similar mass transfer. The tracer, which is injected over a finite length of the surface, is assumed to be chemically inert. Its behavior is controlled by a frozen diffusion equation. The assumption of constant density-viscosity product, and unit Schmidt number results in a linear partial differential equation for the seed mass fraction. This is solved analytically in series form by separation of variables, and numerically by a finite difference technique. It is shown that far downstream of the tracer injection region the analytical results reduce to a simple form; namely, the mass concentration profile is proportional to the local shear even in the presence of mass transfer. However, near the tracer injection region, even the first ten terms are insufficient to yield profiles comparable to those produced by the numerical integration scheme.

Nomenclature

C = trace species
D = diffusion coefficient
f = Blasius function with mass transfer
M = total mass rate of injection of trace species
N = eigenfunction with mass transfer
u,v = velocity components along and normal to the surface
x,y = Cartesian coordinates along and normal to the surface
z = transformed similarity variable
ξ,η = similarity variables
λ = eigenvalue
ϕ = mass fraction of tracer in ablating material
ρ = density
μ = coefficient of viscosity
$(\rho v)_w$ = mass transfer at solid surface

Subscripts

e = outer edge of boundary layer
h = trailing edge of injection region
i = leading edge of injection region
w = wall

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I. Introduction

THIS report investigates the problem of seeded boundary layers with mass transfer, i.e., boundary layers into which small amounts of foreign material are injected and used as tracers. Since the tracer is injected from a limited portion of a surface its concentration profile is different from the other species in the boundary layer. In this report we consider the simplest case of this problem, i.e., injection of a tracer into the boundary layer of a flat plate or cone and adopt the frequently employed approximation of constant $\rho\mu$ and unit Schmidt number in the boundary layer. The velocity profile in the ablating boundary layer then is uncoupled from the species equation and is approximated by the solution of the Blasius equation with mass transfer. The distribution of tracer in the boundary layer is described then by a linear nonsimilar diffusion equation whose coefficients depend upon the solution of the momentum equation. The problem thus formulated has been investigated previously in the case of zero blowing where it corresponds to diffusion with variable wall catalyticity, and to heat transfer to a wall with variable temperature.[1] The formulation of the problem with mass transfer is given in Sec. II.

The problem is investigated both numerically and analytically. The numerical solution is given in Sec. III, where the Crank-Nicholson scheme is used to solve the diffusion equation. The analytical approach is given in Sec. IV and follows that used in the nonblowing case by Fox and Libby,[1] in which a series solution in terms of the eigenfunctions of the partial differential equation is constructed. In the present paper, the eigenfunction expansion is extended to the case of large blowing rates. The importance of the analytical solution is that it yields a simple solution for the species profile far downstream where the profile is insensitive to the details of the injection process. In particular, an analytical solution is given for the injection process in which a large amount of tracer is injected over a small area such that a well-defined limit exists. Since the differential equation is linear, more general solutions can then be constructed from this solution. Far downstream, $\xi/\xi_h > 10$, the leading term in the series is proportional to the local shear; and the remaining terms can be neglected. However, near the downstream edge of the injection region this series converges very slowly and even the first ten terms are inaccurate for $\xi/\xi_h < 1.5$. The numerical integration gives accurate results in the vicinity of the injection area and decays to the analytic result downstream. This is illustrated by an example for which $f_w = -0.70711$ and $\xi_h/\xi_i = 1.75$. In addition, the analytical form becomes particularly simple if the region of tracer injection becomes vanishingly small.

II. Formulation

In the typical situation, a tracer is introduced into the boundary layer as an impurity in the ablation material. The diffusion equation for a chemically inert species is

$$\rho u \partial C/\partial x + \rho v \partial C/\partial y = (\partial/\partial y)\rho D(\partial C/\partial y)] \qquad (1)$$

where D is the diffusion coefficient of the seed with respect to the other species in the layer. The coordinates x and y are along and normal to the surface, and u and v are the respective velocity components. If the tracer is introduced as an impurity in the ablation material over the interva $x_i < x < x_h$ as a constant mass fraction ϕ of the ablating material, the conservation of species at the solid surface gives as the boundary conditions

$$\rho D(\partial C/\partial y) = (C - \phi)(\rho v)_w,\ y = 0,\ x_i \leq x \leq x_h \qquad (2)$$

and

$$\rho D(\partial C/\partial y) = C(\rho v)_w,\ y = 0,\ x_h < x \qquad (3)$$

The remaining initial and boundary conditions imposed on the solution are that there is no seedant upstream of x_i; hence

$$C(x,y) = 0 \qquad x_i < x \qquad (4)$$

and at the outer edge of the boundary layer the concentration also vanishes,

$$C(x,\infty) = 0 \qquad (5)$$

The quantity $(\rho v)_w$ is the mass transfer rate on the surface $y = 0$ and this is considered to be known.

Since the problem is linear in C, we may eliminate ϕ by formulating it in terms of C/ϕ. We therefore will take $\phi = 1$ without loss of generality.

Solution of Eq. (1) is simplified if we use the Howarth-Dorodnitsn similarity variables defined as

$$\xi = u_e(\rho\mu)\int_0^x r^{2j}dx,\quad \eta = \frac{u_e r^{2j}}{(2\xi)^{1/2}}\int_0^y \rho dy \qquad (6)$$

where $j = 0$ for the two dimensional case and $j = 1$ and $r = x \sin\alpha$ for the axisymmetric case. The velocity at the outer edge of the boundary layer is u_e, the density ρ, and the coefficient of viscosity μ. The product $(\rho\mu)$ is assumed to be constant throughout. For a two-dimensional or axisymmetric boundary layer with zero pressure gradient the diffusion Eq. (1) in the similarity variables becomes, for unit Schmidt number $S \equiv \mu/\rho D$

$$\partial^2 C/\partial\eta^2 + f\partial C/\partial\eta - 2\xi f'(\partial C/\partial\xi) = 0 \qquad (7)$$

subject to the boundary and initial conditions

$$\begin{aligned} \partial C/\partial\eta &= -f_w(C-1),\ \xi_i < \xi < \xi_h,\ \eta = 0 \\ \partial C/\partial\eta &= -f_w C,\ \xi_h < \xi,\ \eta = 0 \\ C(\xi,\infty) &= C(\xi_i,\eta) = 0 \end{aligned} \qquad (8)$$

The stream function f satisfies the familiar Blasius equation

$$f''' + ff'' = 0 \qquad (9)$$

subject to the boundary conditions

$$f(0) = f_w,\ f'(0) = 0,\ f'(\infty) = 1 \qquad (10)$$

where f_w is a constant related to the mass transfer at the wall:

$$(\rho v)_w r^j = -\frac{f_w}{(2\xi)^{1/2}}\frac{d\xi}{dx} = -f_w\left(\frac{u_e(\rho\mu)}{2}\right)^{1/2}\frac{r^{2j}}{\left[\int_0^x r^{2j}dx\right]^{1/2}} \qquad (11)$$

The total mass rate of injection of seedant which enters the boundary layer M is given by

$$M = \int_{x_i}^{x_h}(2\pi r)^j\phi(\rho v)_w dx = -(2\pi)^j\phi f_w(2\xi_h)^{1/2}\left[1 - \left(\frac{\xi_i}{\xi_h}\right)^{1/2}\right] \qquad (12)$$

The linear partial differential Eq. (7), subject to the boundary conditions will be solved by numerical and analytical methods. The solution depends upon three parameters: the mass transfer rate f_w, the location of the leading edge of the injection port ξ_i and the ratio ξ_i/ξ_h.

III. Numerical Solution

Equations of the form (7) have been studied extensively, but not with blowing, and discontinuous conditions on C. Some simplification is achieved by the introduction of the logarithmic variable,

$$z = \tfrac{1}{2}\ln(\xi/\xi_i),\ \xi/\xi_i = e^{2z},\ 0 < z < \infty \qquad (13)$$

so that the Eq. (7) for the species becomes

$$\partial^2 C/\partial\eta^2 + f\partial C/\partial\eta - f'\partial C/\partial z = 0 \qquad (14)$$

The change in variables is equivalent to using a varying mesh size along the body. This variable would seem to be the natural variable for other nonsimilar boundary-layer calculations since it requires a lesser number of calculations for large ξ. It cannot be used for $\xi_i = 0$, but for that case the similar solution of (7) holds.

The numerical scheme we used is the Crank-Nicolson implicit finite difference scheme[4] in which the η derivatives are average of 3-point formulas while the z derivative is a forward difference. This gives rise to the following simultaneous algebraic equations for the profile:

$$R_j C_{i+1,j+1} + Q_j C_{i+1,j} + P_j C_{i+1,j-1} = S_{i,j} \qquad (15)$$

where

$$\begin{aligned} R_j &\equiv 1 + \tfrac{1}{2}\Delta\eta f_j,\quad Q_j = -2(1 + f'_j\Delta\eta^2/\Delta z) \\ P_j &= 1 - \tfrac{1}{2}\Delta\eta f_j \\ S_{i,j} &= 2(1 - f'_j\Delta\eta^2/\Delta z)C_{i,j} - R_j C_{i,j+1} - P_j C_{i,j-1} \end{aligned} \qquad (16)$$

The subscript i denotes the value of the species at the spanwise station $i\Delta z$ and the subscript j denotes the value of the species in the normal direction $j\Delta\eta$. The concentration C_w is eliminated from the difference equations by a Taylor Series expansion

$$C_1 = C_w + \Delta\eta \left(\frac{\partial C}{\partial \eta}\right)_w + \frac{\Delta\eta^2}{2}\left(\frac{\partial^2 C}{\partial \eta^2}\right)_w \qquad (17)$$

in which the second derivative is found by setting $f' = 0$ and $f = f_w$ in (14) giving

$$\left(\frac{\partial^2 C}{\partial \eta^2}\right)_w + f_w \left(\frac{\partial C}{\partial \eta}\right)_w = 0 \qquad (18)$$

The first derivative is determined by the boundary conditions (8) as

$$(\partial C/\partial\eta)_w = (\delta - C_w)f_w,\ \delta = 1 \quad (0 < z < z_h)$$
$$= 0 \quad (z_h < z) \qquad (19)$$

If Eqs. (18) and (19) are substituted into (17) and solved for C_w we find

$$C_w = \frac{C_1 - \delta f_w \Delta\eta(1 - \frac{1}{2}\Delta\eta f_w)}{1 - \Delta\eta f_w(1 - \frac{1}{2}\Delta\eta f_w)} \qquad (20)$$

This eliminates C_w from the finite difference Eq. (15) giving matrix algebra of the tridiagonal form. The species distribution is found by application of the following algorithm[4]

$$E_{i,1} = \frac{S_{i,1} + \delta\Delta\eta f_w(1 - \frac{1}{2}\Delta\eta f_w)P_1/[1 - \Delta\eta f_w(1 - \frac{1}{2}\Delta\eta f_w)]}{Q_1 + P_1/[1 - \Delta\eta f_w(1 - \frac{1}{2}\Delta\eta f_w)]}$$

$$E_{i,j} = \frac{S_{i,j} - P_j E_{i,j-1}}{Q_j - P_j W_{i,j-1}};\quad 2 \le j \le N$$

$$W_{i,1} = \frac{R_1}{Q_1 + P_1/[1 - \Delta\eta f_w(1 - \frac{1}{2}\Delta\eta f_w)]} \qquad (21)$$

$$W_{i,j} = \frac{R_j}{Q_j - P_j W_{i,j-1}};\quad 2 \le j \le N - 1$$

$$C_{i+1,N} = E_{i,N}$$

$$C_{i+1,j} = E_{i,j} - C_{i+1,j+1}W_{i,j};\quad 1 \le j \le N - 1$$

One first calculates the E and W from $j = 1$ to N, successively, and then finds the C from $j = N$ to 1 successively. The E and W correspond to successive elimination of each C in favor of the one above, and the solution marches from the edge towards the wall. The stream function f for use in Eq. (16) and Eq. (21) is known from the solution of the differential equation Eq. (10).

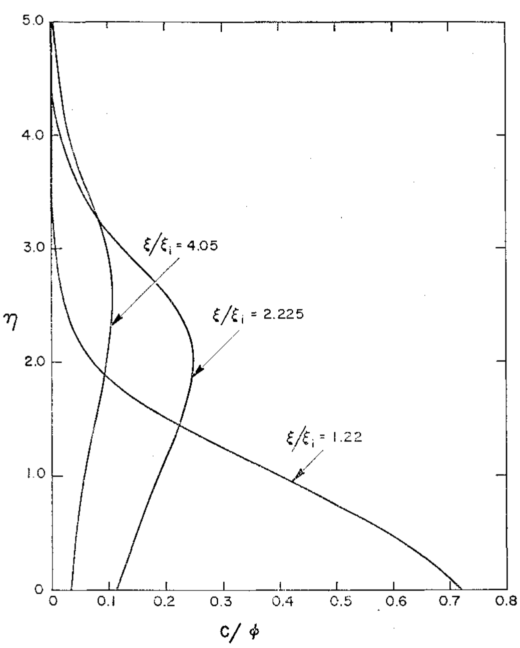

Fig. 1 Species profiles C/ϕ for $f_w = -0.70711$, $\xi_h/\xi_i = 1.75$.

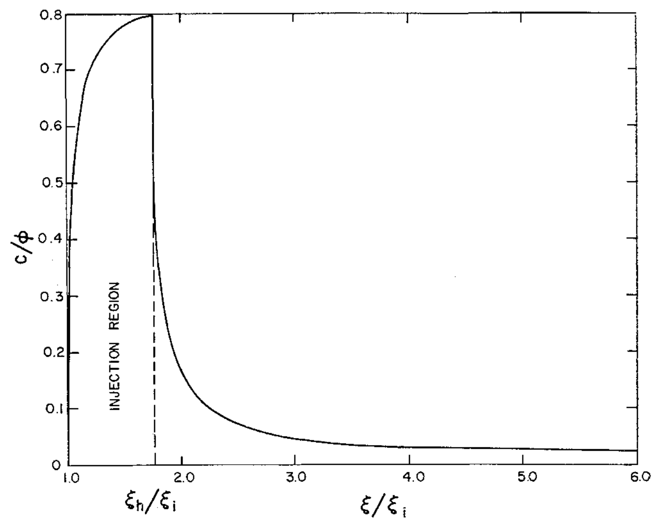

Fig. 2 Species concentration C/ϕ at the wall for $f_w = -0.70711$, $\xi_h/\xi_i = 1.75$.

As an example, the concentration profiles of a typical solution for $f_w = -0.70711$, $f''_w = 0.05024$ are shown in Fig. 1. The injection region was taken to be $\xi_h/\xi_i = 1.75$. The profile at $\xi/\xi_i = 1.22$ is a typical profile in the injection region. All profiles in the injection region have their maximum value at the wall. The profile at $\xi/\xi_i = 2.2$ and 4.0 are typical profiles downstream of the injection region. All profiles in this region have their maximum concentration in the interior of the boundary layer. As ξ/ξ_i increases, this maximum approaches the point of maximum shear of the velocity boundary layer, since as is shown later, $C(\eta)$ becomes proportional to $f''(\eta)$.

The concentration at the wall is shown in Fig. 2. The concentration rises monotonically in the injection region and then decreases very rapidly downstream. It will be shown in the next section that the rate of decrease approaches the $-\frac{1}{2}$ power of the ratio (ξ/ξ_h). Increasing the injection region ξ_h/ξ_i causes the wall concentration in the injection region to approach the value 0.934. This is the value predicted by the similar solution of (7). Otherwise the profiles and wall concentration downstream are of the same form as depicted in Figs. 1 and 2.

The numerical program thus provides a fast and accurate method for finding the distribution of seed in the boundary layer.

IV. Analytical Solution

Since the partial differential Eq. (7) is linear, it is possible to obtain separable series solutions. This approach has been exploited by Fox and Libby[1,2] among others. However, except for the zero blowing case, it was not solved with the present boundary conditions. We will write a general series solution in terms of eigenfunctions and eigenvalues.

A separable solution is written in the form

$$C = N_n(\eta)(\xi/\xi_i)^{-\lambda_n/2} \qquad (22)$$

and substituted into Eq. (7) giving the following equation for $N_n(\eta)$

$$N''_n + fN'_n + f'\lambda_n N_n = 0 \qquad (23)$$

The boundary conditions we chose to determine the λ_n and the N_n are as follows:

$$N_n(0) = 1,\ N'_n(0) + f_w N_n(0) = 0 \qquad (24)$$

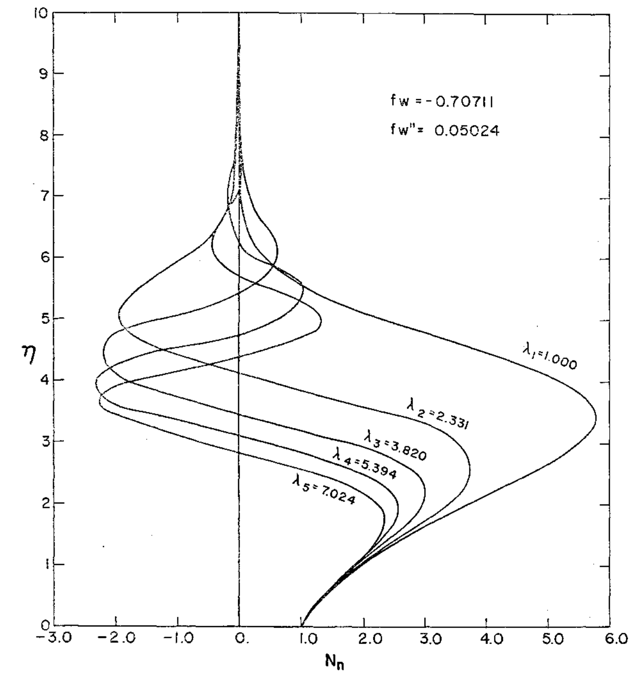

Fig. 3 Eigenfunctions N_n for $f_w = -0.70711$, $n = 1$ to 5.

$$N_n(\infty) = 0 \tag{25}$$

Solutions with exponential decay at infinity exist in particular for discrete values of λ only.

The calculations of λ_n and N_n require integration of (23) starting with the wall conditions (24). The value of λ must be chosen so that $N_n \rightarrow 0$ exponentially as $\eta \rightarrow \infty$. This is a one parameter problem depending on f_w, so we have a one-parameter family of eigenvalues and eigenfunctions, which extends the results of Ref. 1 to nonzero values of f_w.

A numerical scheme for solving this problem is outlined in the Appendix which generates the eigenvalues for a mass transfer rate up to the blow-off limit. For the particular case $f_w = -0.70711, f''_w = 0.05024$ we have obtained the first ten eigenfunctions and eigenvalues, and their norms. The eigenvalues and eigenfunctions are shown in Figs. 3 and 4. It was noticed in the zero blowing case by Fox and Libby[1] that the first eigenvalue is $\lambda_1 = 1$ and the corresponding eigenfunction is

$$N_1 = f''/f''_w \tag{26}$$

This result holds true even with mass transfer. Thus, far downstream, C is proportional to f'' and inversely proportional to $\xi^{1/2}$. One important difference with surface mass transfer is already apparent since the peak concentration is no longer at the wall. Of course, the higher eigenvalues are different from the zero mass transfer results. This comparison is given in Table 1.

The $N_n(\eta)$ are a complete set and any arbitrary function $F(\eta)$ may be expanded as follows‡:

$$F(\eta) = \Sigma A_n N_n(\eta) \tag{27}$$

where the coefficients A_n are given by

$$A_n = \frac{1}{D_n} \int_0^\infty \frac{f' N_n}{f''} F d\eta \tag{28}$$

and the norms D_n by

$$D_n = \int_0^\infty \frac{f' N_n^2}{f''} d\eta \tag{29}$$

‡ All summations run from $n = 1$ to $n = \infty$.

The normalizations D_n are given in Table 1 for the particular case $f_w = -0.70711$. Also presented in Table 1 are results for $f_w = 0$.§ In general for a given accuracy we require more terms of series whenever $f_w \neq 0$. This is due to the relatively slow decrease of the $\lambda_n D_n$.

Having found the separable solutions we now proceed to construct a solution to the seeding problem as follows:

$$C(\xi,\eta) = \int_{\xi_1}^{\xi} \left[C_s(\eta) - \Sigma B_n \left(\frac{s}{\xi}\right)^{\lambda_n/2} N_n(\eta) \right] K(s) ds \tag{30}$$

Here $C_s(\eta)$ is the similar solution of Eq. (7), K is a kernel function to be found, and B_n are coefficients to be determined. The integrand satisfies the differential equation since both $C_s(\eta)$ and $N_n \xi^{-\lambda_n/2}$ do. So when (30) is substituted into (7) the only remaining term comes from differentiation of the upper limit and evaluation of the integrand there. This must vanish to satisfy (7) giving

$$C_s(\eta) - \Sigma B_n N_n(\eta) = 0 \tag{31}$$

The coefficients B_n are just the expansion of the similar solution in terms of the eigenfunctions. The similar solution of Eq. (7) is related to the velocity profile by

$$C_s = (1 - f')/(1 - f''_w/f_w) \tag{32}$$

Substituting (32) into (28) and performing the integration gives for B_n the following:

$$B_n = \frac{(1 - f_w/f''_w)}{(1 - f''_w/f_w) D_n \lambda_n} = \frac{(-f_w/f''_w)}{D_n \lambda_n} \tag{33}$$

Now that we have satisfied the differential equation, let us turn to the boundary and initial conditions. The condition $C \rightarrow 0$ at $\eta \rightarrow \infty$ is certainly satisfied by each term of (30). The lower limit on the integral is chosen so the initial condition $C = 0$ for $\xi = \xi_i$ is satisfied. The boundary condition on the wall, which we will write with the help of Heaviside step functions as

$$\partial C/\partial \eta + f_w C = f_w [H(\xi - \xi_i) - H(\xi - \xi_h)] \text{ on } \eta = 0 \tag{34}$$

then determines the kernal function $K(\xi)$. Substituting (30) into (34) gives an integral equation for $K(\xi)$. The

Table 1 Eigenvalues and norms for $f_w = -0.70711$, $f''_w = 0.05024$

n	λ_n	D_n	$(\lambda_n D_n)^{-1}$
1	1.000	198.11	0.005048
2	2.331	107.84	0.003980
3	3.820	84.72	0.003090
4	5.394	74.92	0.002474
5	7.024	69.78	0.002040
6	8.692	66.77	0.001723
7	10.390	64.87	0.001484
8	12.111	63.64	0.001297
9	13.851	62.82	0.001149
10	15.605	62.28	0.001029
Eigenvalues and norms for $f_w = 0, f''_w = 0.469600$			
1	1.000	2.267	0.4409
2	2.774	3.184	0.1132
3	4.629	3.772	0.05727
4	6.513	4.219	0.03639
5	8.414	4.586	0.02592
6	10.326	4.903	0.01975
7	12.247	5.182	0.01576
8	14.173	5.435	0.01298
9	16.104	5.665	0.01096
10	18.040	5.878	0.0009430

§ The values of λ_n are almost exactly the same as those given in Ref. 1. The norms D_n are slightly different, by up to a few percent.

solution is given in terms of delta functions

$$K(\xi) = \delta(\xi - \xi_i) - \delta(\xi - \xi_h) \tag{35}$$

After integration by parts we have for the species the following results:

$$C = \Sigma B_n[1 - (\xi_i/\xi)^{\lambda_n/2}]N_n(\eta),\ \xi_i \leq \xi \leq \xi_h \tag{36}$$

$$C = \Sigma B_n N_n(\eta)[(\xi_h/\xi)^{\lambda_n/2} - (\xi_i/\xi)^{\lambda_n/2}],\ \xi > \xi_h \tag{37}$$

It can be verified that (36) and (37) do indeed satisfy the differential equation and boundary conditions. It is remarkable that only the expansion of the similar solution C_s is required for the series solution.

We may use Eq. (12) to express the B_n in terms of the total mass flux M instead of the lowing parameter f_w

$$B_n = \frac{M}{(2\pi)^j} \frac{1}{f''_w D_n \lambda_n} \frac{1}{(2\xi_h)^{1/2}[1 - (\xi_i/\xi_h)^{1/2}]} \tag{38}$$

This leads to the possibility of an interesting limit where M is fixed while $\xi_i \to \xi_h$. Combination of (38) with (37) in this limit yields

$$C = \frac{M}{(2\pi)^j f''_w (2\xi_h)^{1/2}} \sum \frac{N_n(\eta)}{D_n}\left(\frac{\xi_h}{\xi}\right)^{\lambda_n/2} \tag{39}$$

One example has been worked out in detail, namely $f_w = -0.70711$ corresponding to the numerical example given in Sec. III. The question of rapidity of convergence of these various series solutions has not been touched on. Previous experience[1,2] would suggest they are slowly convergent, and one needs many terms for an accurate solution. We compared the series solution with the numerical one using ten terms of the series (36) and (37). Table 2 shows these results. Using ten terms of the series solution gives excellent results for $\xi/\xi_h > 1.5$ but is less accurate at the end of the short injection region $\xi/\xi_h = 1.0$. For $\xi/\xi_h > 10$ only the first term of the series is required for accuracy of the order of 5%.

In the limit $\xi_h \equiv 0$ Eq. (39) reduces to one term and can be used to determine the concentration in the boundary layer for any species generated at the stagnation point of a slightly blunted cone. In that case M given by (12) is replaced by the integrated species flux at the stagnation point. For a cone the species concentration decays as $x^{-3/2}$ and the concentration profile in the boundary layer is proportional to the shear profile.

V. Conclusions

A simple problem has been studied in which a tracer is injected into a self-similar mass transfer boundary layer of a flat plate or cone. The velocity boundary layer for the zero pressure gradient case is selfsimilar, satisfying the Blasius equation with mass transfer. The tracer is injected over a finite length of surface as a constant mass fraction of the mass transfer material, and is assumed not to react with the rest of the gas present.

This problem has two physical parameters: 1) the blowing parameter f_w, and 2) the geometric parameter giving the ratio of seeding region size to location. This mathematical problem has been attacked both numerically and analytically. Numerical solutions are easily obtained and show that the concentration profile becomes proportional to the shear far downstream of the seeding region.

Since the differential equation is linear, series solutions are also obtained, following ideas set forth, for example, by Fox and Libby[1] in the zero mass transfer case. This is carried through in Sec. IV in terms of eigenvalues and eigenfunctions. The series solutions are valid in both the injection region and downstream. However, the series solutions converge slowly near the injection region and an example shows that even 10 terms are insufficient to give reasonable agreement with the numerical solution. The importance of the analytical solution lies in the fact that results far downstream of the injection region are easily determined without resort to a numerical solution since only the first term in the series is required. This term shows the concentration to be proportional to the shear, so that the maximum concentration of species far downstream of the injection region occurs at a point of maximum shear of the velocity boundary layer. For a boundary layer with mass transfer this maximum is in the interior of the boundary layer.

Table 2 Comparison of analytical and finite difference solutions $f_w = -0.70711$, $f''_w = 0.05024$, $\xi_h/\xi_i = 1.055$

	$C(\xi/\xi_h = 1.0)$		$C(\xi/\xi_h = 1.5)$	
η	10 terms analytical	Finite difference	10 terms analytical	Finite difference
0	0.04160	0.5485	0.01306	0.01312
0.4	0.05493	0.4100	0.01727	0.01688
0.8	0.07041	0.2488	0.02240	0.02182
1.2	0.08458	0.1096	0.02787	0.02685
1.6	0.09065	0.0289	0.03233	0.03048
2.0	0.07971	0.0039	0.03366	0.03068
2.4	0.04695	0.0002	0.02977	0.02603
2.8	0.00234	...	0.02056	0.01752
3.2	−0.02672	...	0.00958	0.00873
3.6	−0.01911	...	0.00226	0.00300
4.0	0.00706	...	0.00049	0.00067
4.4	0.01301	...	0.00078	0.00009
4.8	−0.00143	...	0.00020	0.00001

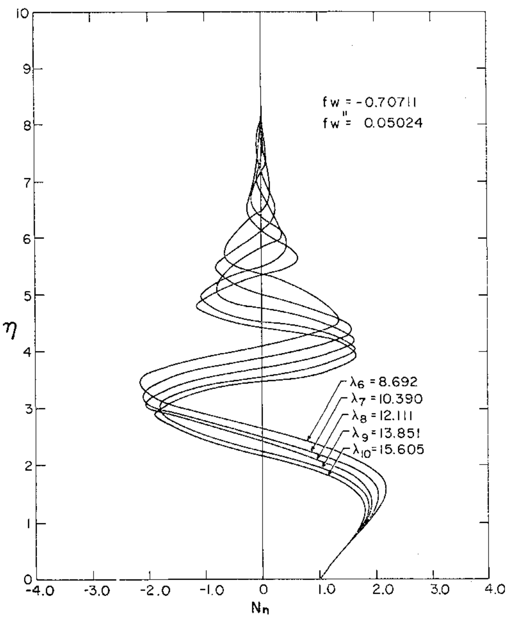

Fig. 4 Eigenfunctions N_n for $f_w = -0.70711$, $n = 6$ to 10.

Appendix

Solutions with exponential decay are more easily found by setting

$$Z_n = N_n \exp\left(\frac{1}{2}\int_0^\eta f d\eta\right) = \left(\frac{f''_w}{f''}\right)^{1/2} N_n \tag{A1}$$

which transforms (23) into

$$Z'' + [(\lambda - \tfrac{1}{2})f' - f^2/4]Z(\eta) = 0 \tag{A2}$$

subject to

$$Z(0) = Z_w = 1,\ Z'(0) = Z'_w = \tfrac{1}{2}f_w,\ Z(\eta \to \infty) \to 0 \tag{A3}$$

We may start integrating from $\eta = 0$, but must choose λ so that the condition as $\eta \to \infty$ is satisfied. One solution of (A2) is exponentially decreasing while the other is exponentially increasing and we must find a way to eliminate the increasing solution.

This sort of problem is conveniently solved by a method put forward by Nachtsheim and Swigert.[6] They suggest that at $\eta \to \infty$ all derivatives of Z vanish, but at any finite η this is not true. Thus, a good error criterion at a finite η is *both* Z and Z' near zero. (All other derivatives would then be small also.) However, with only one parameter, λ at our disposal, we cannot satisfy both these criteria separately, and they propose using the sum of the squares of the deviations from the desired values as an error criterion

$$E^2 = Z^2 + (Z')^2 \qquad \text{(A4)}$$

The idea is to minimize this error at any finite η at which the integration is stopped.

Suppose the integration with some value of λ has been carried to a value of η, say η_s, where the values Z, Z' are obtained. If we now wish to reduce E^2 at this η_s we may change λ by an amount $\Delta\lambda$, which would change Z and Z', in a linear approximation to

$$Z + Z_\lambda \Delta\lambda, \quad Z' + Z'_\lambda \Delta\lambda \qquad \text{(A5)}$$

where Z_λ, Z'_λ are partial derivatives with respect to λ of Z, Z' at the η_s under consideration. They can be defined because Z may be thought of as a function of both η and λ.

We wish to make a change in λ which will minimize the sum of the squares of the two expressions in (A5). Taking the derivative of that sum with respect to $\Delta\lambda$, equating to zero, and solving for $\Delta\lambda$ we find

$$-\Delta\lambda = \frac{ZZ_\lambda + Z'Z'_\lambda}{Z_\lambda^2 + (Z'_\lambda)^2} \qquad \text{(A6)}$$

If we make this change in λ and integrate again to η_s the linear approximation says the *new* Z,Z' will have a minimum square error. This will only be true in actuality if $\Delta\lambda$ is very small, but if we repeat the process again and again, each time changing λ by (A6), we might hope to get smaller and smaller $\Delta\lambda$, and have the resulting E^2 approach a minimum. In fact, if we calculate the minimum of E^2 with respect to λ from (A4) we find the required condition is

$$ZZ_\lambda + Z'Z'_\lambda = 0 \qquad \text{(A7)}$$

which is just the statement that $\Delta\lambda = 0$. Thus as we approach a minimum E^2 for repeated integrations to a given η_s with improved λ, $\Delta\lambda \to 0$. There is of course an irreducible minimum E^2 which one can reach at any η_s, but this minimum approaches zero monotonically as $\eta_s \to \infty$.

The idea is now clear. Beginning with a guess for λ, we integrate out to some η_s, compute a change in λ by applying (A6) at that point, and reintegrate with the new λ. When the changes in λ get very small we integrate to a larger η_s and repeat. The process stops when a small enough value of E^2 is reached, or by some other suitable criterion. In effect we "sneak" up on the solution from the $\eta = 0$ side. This procedure is particularly suited to equations which have unwanted exponentially growing solutions, since one may march out in small enough steps in η_s to prevent the solution from "blowing up."

The partial derivatives needed in (A6) can be obtained several ways. For complicated equations one may merely integrate with two closely spaced values of λ and use the difference form of the derivative. For an equation as simple as ours we may differentiate (A2) and (A3) with respect to λ, to get

$$Z''_\lambda + [(\lambda - \tfrac{1}{2})f' - f^2/4]Z_\lambda + f'Z = 0 \qquad \text{(A8)}$$

$$Z_\lambda(0) = 0, \; Z'_\lambda(0) = 0$$

The latter follow from the fact that the boundary conditions are independent of λ (as are f and f'). This is an inhomogeneous second-order equation in Z_n with homogeneous boundary conditions, and is coupled to (A2) through the $f'Z$ term. They are to be solved simultaneously.

This procedure was carried out, and at the same time calculations of N and D were carried along. In fact, since the norm D was of primary interest, we used as an error criterion the constancy of D to one part in 10^{-5}. When this was achieved as η changed, we stopped the integration.

As a test, this procedure reproduced $\lambda_1 = 1$ to 6 figures and D_1 to the accuracy of the input, which was $f''_w = 0.05024$ for $f_w = -0.70711$.

Of course, it helps to have a good guess for λ, and a set of guesses was obtained by a finite difference scheme. Equation (A2) was expressed in finite difference form using a 3-point formula for Z''. The result is

$$Z_{j-1} + [(\lambda - \tfrac{1}{2})\Delta\eta^2 f'_j - 2 - \Delta\eta^2 f_j^2/4]Z_j + Z_{j+1} = 0 \qquad \text{(A9)}$$

The boundary conditions are handled just as described in Sec. IV for the partial differential equation. The outer one is $Z_{N+1} = 0$, the inner obtained by Taylor series using the differential equation and wall conditions to express the value $Z(0) = Z_w$ as

$$Z_w = Z_1/[1 - \tfrac{1}{2}\Delta\eta f_w(1 - \Delta\eta f_w/4)] \qquad \text{(A10)}$$

If (A9) is written for $j = 1, 2, \ldots N$, and $Z_{N+1} = 0$ and Z_w given by (A10) used, we have N homogeneous equations in N unknowns $Z_1, Z_2, \ldots Z_N$. The determinantal condition for a nontrivial solution is an Nth-order equation for λ which gives N approximations to the eigenvalues. The determinant is tridiagonal and easy to solve for the λ_n.

This procedure was used with $\Delta\eta = 0.1$, $N = 100$, to find approximate values of λ_n. It was found that the first few were quite accurate, the first being 0.99887 for the aforementioned case, but they got less accurate as η got larger.

It seems clear this method is excellently suited for solving difficult two-point boundary value problems by forward integration, and avoids all the complications associated with quasi-linearization (it works as well on nonlinear equations), integration in from large η, etc. As Ref. 6 shows, it works the same way when one of the boundary conditions at $\eta = 0$ is the unknown instead of a parameter in the equation, and for systems of equations with several unknowns.

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