VARIATIONAL APPROXIMATION FOR THE STRUCTURE OF A DIFFUSION FLAME

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An approximation for the structure of a diffusion flame was obtained by means of the Rayleigh-Ritz method. The results are simple and illustrate the various features of interest in the flame problem. The accuracy of the approximation is discussed.

This paper deals with an approximate solution for the following differential equation and boundary conditions:

$$\frac{d^2\Lambda}{dx^2} = (\Lambda - z)^{\chi}(\Lambda + z)^{f} \qquad \text{Eq. 1}$$

$$\Lambda \sim z, \quad z \to \infty$$
$$\Lambda \sim -z, \quad z \to -\infty \qquad \text{Eq. 2}$$

In this problem, Λ is related to either the oxidant or fuel concentration in a diffusion flame, or the associated temperature distribution. The independent variable z is related to the coordinate normal to the flame. The symbols χ and f denote the stoichiometric coefficients (integers) for the irreversible oxidant-fuel-product reaction

$$\chi X + f F \to gP \quad , \qquad \text{Eq. 3}$$

where X, F, and P represent the oxidant, fuel, and product species, and g the stoichiometric coefficient for the product species. For two dimensional steady flows, the coordinate measured along the flame appears as a parameter in both the variables Λ and z (1, 2, 3). For one dimensional unsteady flows, the time appears as a parameter in Λ and z (4). The oxidant lies on the negative ($z < 0$) side of the flame and the fuel on the positive ($z > 0$) side, and the flame exists at the interface where these two species diffuse into one another and combine chemically according to Eq. 3. Further background on this problem can be found in a review article by Williams (5).

Owing in part to the nonlinear character of Eq. 1, no exact solution has been found. Moreover, because the equation and boundary conditions constitute a two-point boundary-value problem over an infinite domain, a numerical integration is altogether not a trivial matter. However, numerical solutions have been obtained for $\chi = f = 1$ (1, 2) and for $\chi = 1, f = 2$; $\chi = f = 3$; and $\chi = 1, f = 5$ by Chung *et al.* (6) Unfortunately the numerical results of Chung et al. are plotted to such small scales and in such a way that precise values cannot be ascertained, and only the roughest trends can be discerned. It would be very useful to have an approximate solution, simple in form, that reflects the trends involved when χ and f are varied, and especially the asymmetrical behavior that occurs when χ and f are not equal. Such an approximate solution would provide a means of making rapid calculations and lead to a better understanding of the problem. This investigation is directed towards obtaining such an approximation by means of the Rayleigh-Ritz method. Besides obtaining information about the mathematical problem itself, we wish to evaluate the accuracy and utility of the Rayleigh-Ritz method for these types of problems.

Variational Formulation

Following Hildebrand (7) we establish the variational formulation of the problem by multiplying Eq. 1 by the variation $\delta\Lambda$ and the differential dz and integrating over all z:

$$\int_{-\infty}^{\infty} [\Lambda'' - (\Lambda - z)^{\chi} (\Lambda + z)^{f}] \, \delta\Lambda dz = 0 \qquad \text{Eq. 4}$$

Integrating the first term by parts and imposing the condition $\delta\Lambda = 0$ at the end points $z \to \pm\infty$ leads to

$$\delta I = 0 \qquad \text{Eq. 5}$$

where

$$I = \int_{-\infty}^{\infty} [\tfrac{1}{2}(\Lambda'')^2 + G(\Lambda, z)]\, dz \qquad \text{Eq. 6}$$

and

$$G(\Lambda, z) = \int_{|z|}^{\Lambda} (\lambda - z)^{\chi} (\lambda + z)^{f}\, d\lambda - \tfrac{1}{2} \qquad \text{Eq. 7}$$

The function of integration in G (Λ,z) was selected so that the integral I is finite. Eq. 5 asserts that $\Lambda(z)$ is the function that makes the integral I stationary. Further considerations show that I is a minimum.

The underlying idea of the Rayleigh-Ritz approximation is discussed by Hildebrand (7). The idea is to select a trial function for $\Lambda(z)$ that satisfies the boundary conditions, but one with free constants available to be determined such that I is stationary for that function. Before choosing a trial function, it is useful to examine the asymptotic behavior of the exact function $\Lambda(z)$.

Asymptotic Behavior

In order to choose and evaluate a trial function for the Rayleigh-Ritz approximation, it is useful to understand the asymptotic behavior of the exact solution for large z. For large positive z, we write

$$\Lambda \sim z + F, \qquad \text{Eq. 8}$$

where F is small compared to z. Eq. 1 then shows that F behaves asymptotically as

$$F'' \sim (2z)^{f} F^{\chi}. \qquad \text{Eq. 9}$$

Clarke (8) discussed this asymptotic behavior and obtained

$$F \sim \left[m(m-1)2^{-f}\right]^{1/(\chi-1)} z^{m}, \chi > 1,\ f \geq 1, \qquad \text{Eq. 10}$$

where $m = -\frac{f+2}{\chi-1}$,

and

$$F \sim A\, z^{-f/4} \exp\left\{-\frac{(2z)^{(2+f)/2}}{2+f}\right\}, \chi = 1,\ f \geq 1, \qquad \text{Eq. 11}$$

where A is an arbitrary constant. When z is negative and large, corresponding results were obtained with χ and f interchanged from above. When z is positive and large, F vanishes algebraically when $\chi > 1$ and exponentially when $\chi = 1$. We also note that an arbitrary constant is present only when $\chi = 1$ since then Eq. 9 is linear.

Rayleigh-Ritz Approximation

We choose the following piecewise continuous function:

$$\begin{aligned} \Lambda &= -z + a^{-1} e^{b_1 z}, & z \leq 0 \\ \Lambda &= z + a^{-1} e^{-b_2 z}, & z \geq 0 \end{aligned} \qquad \text{Eq. 12}$$

We further require that the derivative Λ is continuous at $z = 0$. This leads to

$$a = \tfrac{1}{2}(b_1 + b_2) \qquad \text{Eq. 13}$$

There are thus two constants to be determined, b_1 and b_2. This choice of function satisfies the boundary conditions, is simple, and allows for an asymmetric behavior for arbitrary values of χ and f. We can see from Eqs. 10 and 11 that, when z is large and positive, the exponential part of Eq. 12 dies out too slowly when $\chi = 1$ and too rapidly when $\chi > 1$. Nevertheless it has an overall simplicity and shows a more accurate representation overall than an alternate function with the correct asymptotic behavior which will be discussed later.

Following Hildebrand (7) we determine the variation of Λ in terms of δb_1 and δb_2 and substitute $\delta\Lambda$ and Λ into Eq. 4. The coefficient of δb_1 and δb_2 must vanish independently. This provides two equations for b_1 and b_2, which can be expressed as

$$\begin{aligned} 3a^{1+\chi+f} &= 2A_1 \int_0^{\infty} (1+2A_1 y)(2A_1 y + e^{-y})^{\chi} e^{-(1+f)y} dy \\ &\quad + 2A_2 \int_0^{\infty} (2A_2 y + e^{-y})^{f} e^{-(1+\chi)y} dy \end{aligned} \qquad \text{Eq. 14}$$

$$A_1^2 \int_0^{\infty} y(2A_1 y + e^{-y})^{\chi} e^{-(1+f)y} dy = A_2^2 \int_0^{\infty} y(2A_2 y + e^{-y})^{f} e^{-(1+\chi)y} dy \qquad \text{Eq. 15}$$

where $A_1 \equiv a/b_1$ and $A_2 \equiv a/b_2$. Since

$$A_2 = A_1/(2A_1 - 1), \qquad \text{Eq. 16}$$

Eq. 15 amounts to a single equation for A_1 or A_2. After it has been solved, the right-hand side of Eq. 14 can be evaluated and the constant a determined, whence b_1 and b_2 can be determined.

For the symmetric case $\chi = f = n$, Eq. 15 yields $a = b_1 = b_2$, and Eq. 14 becomes

$$a^{1+2n} = \frac{4}{3} \int_0^{\infty} (1+y)(2y+e^{-y})^n \, e^{-(1+n)y} dy \quad \text{Eq. 17}$$

In this case, Eq. 12 can be written

$$\Lambda = |z| + a^{-1} e^{-a|z|} \quad \text{Eq. 18}$$

For n = 1, 2, 3, we obtain

$$n = 1: \quad a = (52/27)^{1/3} \simeq 1.2441$$

$$n = 2: \quad a = \left(\frac{6521}{4050}\right)^{1/5} \simeq 1.0999$$

$$n = 3: \quad a = \left(\frac{2,363,659}{1,653,750}\right)^{1/7} \simeq 1.0523$$

The minimum value of Λ is a^{-1} and occurs at z = 0. Thus for n = 1,2,3 we obtain Λ_{min} = 0.8038, 0.9092, 0.9503, respectively. The minimum value of Λ increases as n increases.

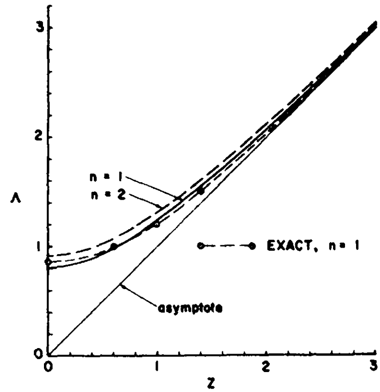

FIGURE 1. Comparison of Rayleigh-Ritz approximations, n = 1, n = 2, with exact values for n = 1.

Figure 1 shows a comparison of the approximations for n = 1 and n = 2 together with the exact values (2) for n = 1. For the exact values, Λ_{min} = 0.8657, and hence the above Rayleigh-Ritz approximation for n = 1 is 7.15% too low at the minimum value, which is the largest error between

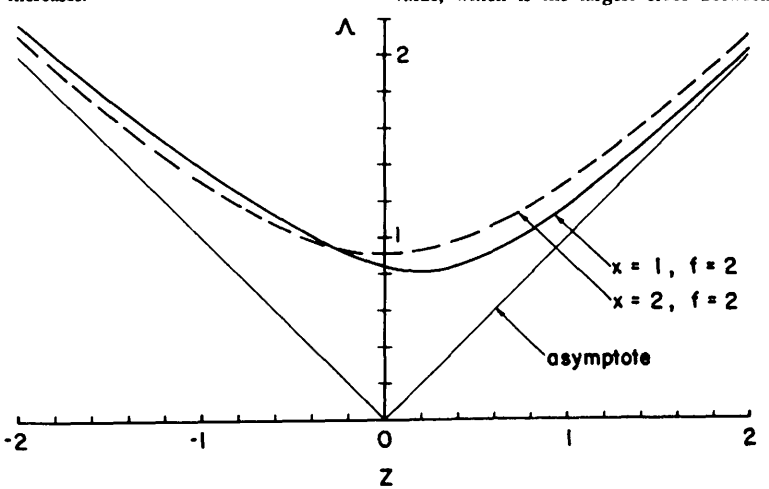

FIGURE 2. Comparison of Asymmetric Curve, $\chi = 1$, f = 2, with symmetric curve, $\chi = f = 2$.

the exact and approximate curves. The approximate curve lies above the exact curve as the asymptote is approached. For such a simple expression given by Eq. 18 the overall agreement with the exact values is good. The curve for $n = 2$ shows the effect of changing the order of the reaction, n.

Consider now the asymmetric results for $\chi = 1$ and $f = 2$. Eq. 15 becomes

$$A_1^2\left[\frac{1}{16} + \frac{4}{27} A_1\right] = A_2^2\left[\frac{1}{16} + \frac{8}{27} A_2 + \frac{3}{2} A_2^2\right] \quad \text{Eq. 19}$$

In view of Eq. 16, this is an algebraic equation for A_1 which can be solved graphically or by other numerical means. We determine that $A_1 = 1.497$ and $A_2 = 0.7508$. It follows from Eq. 14 that $a = 1.190$ and hence that $b_1 = 0.7949$ and $b_2 = 1.585$. These results are plotted in Fig. 2 and compared to the symmetric curve for $n = 2$. The minimum for the asymmetric curve $\chi = 1$, $f = 2$, occurs at $z = 0.181$ and has the value $\Lambda_{min} = 0.8118$. This minimum is closer to the symmetric curve for $n = 1$ than it is for $n = 2$. The asymmetric curve lies below the curve for $n = 2$ for positive z and above the curve for $n = 2$ for negative z.

DISCUSSION

The previous results are simple and general. They show the trends for different values of χ and f, and they are easily obtained. The results are reasonably accurate, at least for the case $n = 1$. We now wish to discuss briefly some alternative functions and some points regarding the accuracy of the Rayleigh-Ritz approximations.

Because of the asymptotic behavior for $\chi > 1$ and $f \geq 1$ when $z \to \infty$, reflected by Eq. 10, a possible trial function for the symmetric case $\chi = f = n > 1$ might be

$$\Lambda = |z| + \frac{1}{sC(1+C|z|)^s} \quad \text{Eq. 20}$$

where $s = (n+2)/(n-1)$. This choice varies algebraically in accordance with Eq. 10, but it cannot be used for $n = 1$. A generalization for the asymmetric case is also possible. By means of the Rayleigh-Ritz procedure an expression for C as a function of s can be obtained, similar to Eq. 17. For $n = 2$, $s = 4$, we obtain $C = 0.2938$. We also obtain $\Lambda_{min} = 0.8509$. A comparison with the algebraic representation, Eq. 20, with the exponential representation, Eq. 18, is shown in Fig. 3 for $n = 2$. Since the

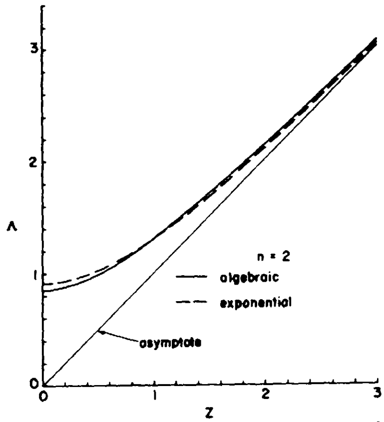

FIGURE 3. Comparison of exponential and algebraic representations for $n = 2$.

exponential representation yielded a value of Λ_{min} that was too low for $n = 1$, it might be expected that this would be true of all values of n. Since the algebraic representation yields a value of Λ_{min} that is lower than that for the exponential representation for $n = 2$, the exponential representation appears to be the better, at least in this regard. A comparison can also be made by calculating the value of the functional I, Eq. 6. The value of I for the exponential representation is $I = -1.1365$ and for the algebraic case $I = -1.1030$. Since I is to be a minimum, we conclude that the exponential formula is a better overall representation. Such a consideration as this must be used when no other information is available.

The exponential representation can be improved by introduction of additional constants to be evaluated. For the symmetric case, we add one more constant and write

$$\Lambda = |z| + b^{-1}(1 + a_1 + a_1 b|z|)e^{-b|z|} \quad \text{Eq. 21}$$

where $\Lambda'(0) = 0$. When $a_1 = 0$ this expression reduces to Eq. 18. We have two constants to evaluate, and for n = 1 the Rayleigh-Ritz approximation gives b = 2.0562 and a_1 = 0.7880. The minimum value is Λ_{min} = 0.8696, which can be compared to the exact value Λ_{min} = 0.8657.

This agreement is very good, and good agreement is also found over the whole range of z. Although better accuracy is obtained, more work is required to evaluate the constants. A generalization to Eq. 21 can be found that holds also for the asymmetric cases.

CONCLUDING REMARKS

The Rayleigh-Ritz method is a viable means for obtaining approximate solutions for diffusion-flame structure. The results are simple, accurate, and demonstrate the trends associated with variations in χ and f. The method could prove useful also in diffusion-flame problems that involve more complicated chemistry.

REFERENCES

1. A. LINAN, *On the Structure of Laminar Diffusion Flames*, Ph.D. Thesis, Calif. Inst. Tech., Pasadena, California, 1963.
2. F. E. FENDELL, J. Fluid Mech. 21: 281-303 (1965).
3. J. F. CLARKE, J. Inst. Maths. Applics. 3: 347-361 (1967).
4. M. L. RASMUSSEN, *Diffusion Flames Associated with Weak Explosions*, Aero Report 2-74, Cranfield Institute of Technology, Aerodynamics Division, Cranfield, Bedford, England, 1974.
5. F. A. WILLIAMS, Ann. Rev. Fluid Mech. 3: 171 (1971).
6. P. M. CHUNG, F. E. FENDELL, and J. F. HOLT, AIAA J. 4: 1020-1026 (1966).
7. F. B. HILDEBRAND, *Methods of Applied Mathematics*, 2d Edition, Prentice-Hall, Inc., New Jersey, 1965. p. 181-193.
8. J. F. CLARKE, J. Eng. Math. 5: 179-185 (1971).