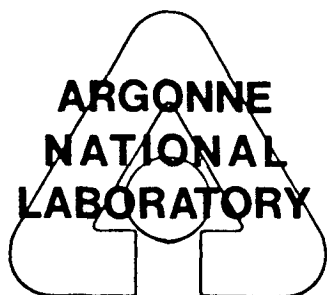# ARGONNE NATIONAL LABORATORY

A NUMERICAL STUDY OF A ONE-STEP FLAME IN A ONE-DIMENSION GAS

by

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ABSTRACT

We consider a diffusional thermal model of a flame in a one-dimensional premixed combustible gas. The flame results from a one-step reaction governed by Arrhenius kinetics. The equations are solved using a general purpose nonlinear PDE solver which uses the Galerkin method and B-splines. In particular we concern ourselves with the character of the flame as a function of the Lewis number. An analysis by Matkowsky and Olagunju, based on a similar model, indicated that the Lewis number acts as a bifurcation parameter where the basic solution is a flame propagating with constant velocity and the bifurcated solution propagates in an oscillatory fashion.

1. Introduction

The problem of a flame in a one-dimensional premixed combustible gas was studied analytically by Matkowsky and Olagunju [1]. In their analysis the flame is presumed to result from a one-step reaction governed by Arrhenius kinetics, i.e.:
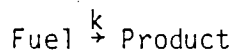
$$\text{Fuel} \xrightarrow{k} \text{Product}$$
$$k = Ze^{-E/RT}$$

Z = preexponential factor

E = activation energy

R = universal gas constant

The equations modelling this flame are derived in a paper by Matkowsky and Sivashinsky [2]. Among other things they assume small thermal expansion to decouple the equations of fluid dynamics from the full equations of combustion theory and large activation energy which implies a narrow reaction zone and thus allows the Arrhenius reaction term to be replaced by a delta function multiplied by an appropriate constant.

In order to study the behavior of the flame numerically and to compare our results with those obtained by Matkowsky and Olagunju, we selected a similar model in which the Arrhenius reaction term is not replaced by the computationally awkward delta function.

2. The Analytic Results

Matkowsky and Olagunju concluded that the Lewis number, a ratio of the thermal conductivity to the coefficient of diffusion, acts as a bifurcation parameter. There is a critical Lewis number, L_c, such that for $L < L_c$ the solution takes the form of a uniformly propagating flame front and at $L = L_c$ a second solution bifurcates supercritically from this basic solution. The second solution is a flame that pulsates forward. A stability analysis indicated that for $L > L_c$ the basic solution is unstable and so it was conjectured that the oscillatory solution would be observed. The critical Lewis number is a function of the activation energy, N, and the temperature of the incoming unburnt fuel, σ. Mathematically:

$$L_c = 1 + 4(1+\sqrt{3})\left(\frac{1}{N(1-\sigma)}\right) + 0\left(\frac{1}{\{N(1-\sigma)\}^2}\right)$$

The amplitude of the pulsations increases with the Lewis number for L close to L_c. Introducing ε as a measure of how much L exceeds L_c, they obtained the following formula for the velocity of the flame front as a function of time:

$$u(t) = -1 - (\omega_0 \sin \omega_0 t)\varepsilon + \omega_0(2b_3 \cos 2\omega_0 t - 2a_3 \sin 2\omega_0 t + k)\varepsilon^2$$
$$+ 0(\varepsilon^3)$$

where
$$\varepsilon \approx \sqrt{N(1-\sigma)(L-L_c)/\beta_2}$$
$$\omega_0 \approx 0.636$$
$$a_3 \approx -0.142$$
$$b_3 \approx 0.3$$
$$k \approx 0.046$$
$$\beta_2 \approx 0.465$$

In Figures 1, 2, and 3 the absolute value of this function is plotted against time for $\varepsilon = 0.3$, 0.6, and 1.0, respectively. The graph of $\varepsilon = 1.0$ introduces the possibility of a second major change in the flame behavior from a singly to a doubly periodic solution. Whether or not this actually occurs, either through the above mechanism or as a result of a secondary bifurcation, is an open question.

3. The Numerical Model

As mentioned above, the principle difference between the two models is that in our model we have preserved the Arrhenius reaction term:

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} = \frac{1}{L} \frac{\partial^2 C}{\partial x^2} - W(C,T)$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} = \frac{\partial^2 T}{\partial x^2} + (1-\sigma)W(C,T)$$

$$W(C,T) = A(1-\sigma)^2 N^2 C e^{N(1 - 1/T)}$$

$$x \quad [-20,40], \quad t \geq 0$$

Boundary Conditions:

$$\left.\frac{\partial C}{\partial x}\right|_{x=-20} = \left.\frac{\partial C}{\partial x}\right|_{x=40} = 0$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=-20} = \left.\frac{\partial T}{\partial x}\right|_{x=40} = 0$$

Initial Conditions:

$$C(x,0) = \begin{cases} 1-e^{k_1 x} & x \leq 0 \\ 0 & x > 0 \end{cases}$$

$$T(x,0) = \begin{cases} \sigma+(1-\sigma)e^{k_2 x} & x \leq 0 \\ 1 & x > 0 \end{cases}$$

C = C(x,t) = concentration of the fuel
T = T(x,t) = temperature of the gas
u = velocity of the gas
L = Lewis number
N = 40 = activation energy
A = 0.5 = preexponential factor
σ = 0.5 = temperature of incoming unburnt gas
k_1 = 3
k_2 = 1

All quantities have been nondimensionalized.

The convection velocity, u, functions as a change of coordinates of the form x' = x-ut, and was chosen to prevent the flame from drifting towards either boundary. The choices of N = 40, A = .5, and σ = .5, correspond to some hypothetical gas. The analysis predicts unit flame speed when A = 0.5. The activation energy, N, was chosen large to match the analysis.

We draw the reader's attention towards the choice of boundary condi-

The initial conditions imply that at t = 0.0 seconds the flame is located at x = 0.0. For x > 0.0 the concentration is zero and the temperature is unity, thus the flame has travelled through this zone depleting the fuel and increasing the temperature. For x < 0.0 the concentration increases exponentially to unity and the temperature to σ, both values associated with the fresh combustible mixture.

The constants k_1 and k_2 control the overlap of the initial concentration and temperature profiles. The overlap is that region where the temperature is high and the concentration is not negligible. Increasing k_1 steepens the concentration profile and therefore increases the overlap. Increasing k_2 steepens the temperature profile which decreases the overlap. If the profiles overlap too much then the flame will 'over-ignite' resulting in a prolonged transient period. If there is insufficient overlap then the flame fails to ignite and the temperature and concentration profiles diffuse nearly independently. Our experience has been that, with the exception of the case of non-ignition, the long-time response is insensitive to the initial conditions.

We solved these equations using a general purpose nonlinear partial differential equation solver which uses the Galerkin method and B-splines. In effect this causes a space-variable discretization and reduces the problem to a system of first order ordinary differential equations in the time variable. This system is then solved by another software package which

dynamically adjusts the time step to satisfy certain prescribed minimum error requirements. The PDE solver produces spline coefficients and thus the solution at discrete user specified time points. It interpolates as necessary to obtain values between each of the ODE time points.

We chose to use a fourth-order spline approximation and a continuity index of two. Thus cubic polynomials are strung between each pair of mesh points and the function and its derivative are continuous at the mesh points. Between each pair of mesh points there are four quadrature points and mesh points were placed every 0.1 units over the travel of the flame.

4.   The Numerical Results

Figure 4 is a snapshot taken at t = 23.5 seconds from a run with L = 1.5. (The word "seconds" is used throughout to indicate time even though time has been nondimensionalized.) Species 1 refers to the concentration and species 2 refers to the temperature (labelled "u-axis"). Note that this is a blowup, the actual boundaries are located far to the left at x = -20 and to the right at x = 40.

In Figure 5 a number or profiles are superimposed. A time period of 1.0 to 23.0 seconds is covered in steps of 0.5 seconds during which time the flame moves from left to right under the influence of a convection velocity u = 1.3 units/second. Relative to the gas the flame is actually travelling from right to left at about 1.28 units/second. There are no visible pulsations at this Lewis number (L = 1.5). In Figure 6, the speed of the front is plotted against time. The speed versus time plots are based on the motion of the point on the temperature profile where T = 0.85. Other criteria, e.g., T = .97, yielded similar plots. Since the flame profiles are available only at discrete times, typically every 0.5 seconds, the sharp peaks of the flame speed are often squared off. All speed vs. time plots are adjusted for the convection velocity and therefore show what the flame speed would have been had the flame been moving through a stationary gas.

Figure 7 is a run of L = 1.80. This also appears to be below the critical Lewis number. Pulsations are present but die out exponentially. At L = 1.81 (Figure 8) the pulsations die out with time but the rate of decay is slower.

In Figure 9, L = 1.83. This is evidently greater than L_c as the pulsations to not attenuate but rather increase in amplitude to some constant value. This plot is actually composed of two runs, from 0 to 50 seconds and from 50 to 100 seconds. The latter 50 seconds were run with a smaller time step in order to follow the sharp peaks better.

At L = 1.85 (Figure 10) the amplitude of the pulsations has increased significantly, enough so as to require rescaling the speed axis. The increased amplitude makes it more difficult to follow the peaks and so the tops vary in height. A more likely interpolation is shown in Figure 11.

The numerical results are in qualitative agreement with the analytic results. The fact that they do not agree exactly is probably due to the fact that the analytic formulae are asymptotically valid and were derived under assumptions we do not satisfy, e.g. $N(1-\sigma)^2 \ll 1$ and $L-1 \ll 1$, rather than to the different reaction terms.

Quantitatively, the numerical results suggest $L_c = 1.82$ while using the first two terms of the analytic formula:

$$L_c = 1 + 4(1+\sqrt{3})\left(\frac{1}{N(1-\sigma)} + 0\left(\frac{1}{\{N(1-\sigma)\}^2}\right)\right)$$

yields $L_c = 1.5$. The neglected term may, of course, be large. Indeed Margolis [3] has obtained an additional term using a different model:

$$L_c = 1 + 2(1+\sqrt{3})\left(\frac{1}{N^*}\right) + (13+4\sqrt{3})\left(\frac{1}{N^*}\right)^2 + 0\left(\frac{1}{N^*}\right)^3$$

or, in our variables: $(N^* = N(1-\sigma)/2)$

$$L_c = 1 + 4(1+\sqrt{3})\left(\frac{1}{N(1-\sigma)}\right) + 4(13+4\sqrt{3})\left(\frac{1}{\{N(1-\sigma)\}^2}\right) + \ldots$$

which yields $L_c = 1.75$.

The analysis predicts sinusoidal pulsations with a period of about 10 seconds. In contrast, our pulsations have more of the character of a relaxation oscillation and a period of about 5 seconds. Thus we have characterized the behavior of the flame for $1 < L < 1.85$. As mentioned above, these results were obtained using mesh points every 0.1 units over the travel of the flame.

Fuel for speculation about the behavior of the flame at larger Lewis numbers is provided by previous results obtained with a larger mesh width. With mesh points placed every 0.5 units we found that at L = 1.5 a uniformly propagating flame is observed. At L = 1.55 the flame is pulsating and at L = 1.60 secondary pulsations begin to appear between each of the primary pulsations as in Figure 3. At L = 1.75 these secondary pulsations are approximately as large in amplitude as the primary pulsations. Further increasing L led to more of a spatial structure, see for instance Figure 12 in which L = 2.1. In the neighborhood of the reaction zone a large bump appears concurrently with the advance of the flame front and then diffuses. We note that in reducing the mesh width from 0.5 units down to 0.1 units, the critical Lewis number moves from approximately 1.5 to 1.8. It has been proposed that reducing the mesh width shifts the L-spectrum and thus the same kinds of behavior, including the secondary pulsations, would be seen for larger Lewis numbers with the refined mesh. It is also possible that the coarse mesh has artifically induced the secondary pulsations.

It is interesting to compare the mesh width to the width of the reaction zone. For our purposes, we define the reaction zone by the region between the two points on the temperature profile where T = .976 and T = 1.0. At T = .976 the reaction term, $W = e^{N(1 - 1/T)}$, is approximately $1/e$. In Figure 4, for which L = 1.75, this gives a reaction zone 0.14 units wide.

This thin reaction zone and the associated steepness of the concentration and temperature profiles make necessary a very fine mesh and hence lengthy run times. To a certain extent, this difficulty can be overcome by concentrating mesh points only where they are needed, in the neighborhood of the reaction zone. This can be indirectly accomplished by introducing a stretching of the spatial coordinates as suggested by Butler and O'Rourke [4]. In our scheme we are able to freely position the mesh points but still a large number of mesh points are needed since the reaction zone propagates through space. In this regard, it is very useful to select a convection velocity that stabilizes the position of the flame. A pulsating flame can thus be made to oscillate in place, but the amplitude of the pulsations poses a lower limit on how much the flame travel can be reduced.

Finally, we refer the reader to the work of Grishin, Bertsun, and Agranat [5] and Golovichev, Grishin, Agranat and Bertsun [6]. In [5] the authors used

a different numerical scheme and model to show the existence of pulsations. Their results show a more gradual increase in amplitude and a marked increase in the frequency of pulsations with increasing Lewis number. Basically, we have seen the same behavior over a smaller spectrum of Lewis numbers, though it is not clear from our graphs that the frequency increases with the Lewis number. In [6] a Bromine-Hydrogen flame was simulated numerically with choices of pressure, temperature, etc. that yielded pulsations.

References

[1] Matkowsky, B. J. and Olagunju, D. O., Propgation of a pulsating flame front in a gaseous combustible mixture, SIAM J. Appl. Math., to appear.

[2] Matkowsky, B. J. and Sivashinsky, G. I., An asymptotic derivation of two models in flame theory associated with the constant density approximation, SIAM J. Appl. Math. 37, 686-699 (1979).

[3] Margolis, Stephen B., Bifurcation phenomena in burner-stabilized premixed flames, Combustion Sci. and Tech., 22, 143-169 (1980).

[4] Butler, T. D. and O'Rourke, P. J., A numerical method for two dimensional unsteady reacting flows, Sixteenth Symposium (international) on Combustion, The Combustion Institute of Pittsburgh, PA (1977).

[5] Grishin, A. M., Bertsun, V. N., and Agranat, V. M., Investigation of the diffusional-thermal instability of laminar flames, Dokl. Akad. Nauk. SSSR, 235, 550-553 (1977) = Sov. Phys. Dokl. 22(7), 373-375 (1977).

[6] Golovichev, V. I., Grishin, A. M., Agranat, V. M., and Bertsun, V. N., Thermokinetic oscillations in distributed homogeneous systems, Dokl. Akad. Nauk. SSSR, 241, 305-308 (1978) = Sov. Phys. Dokl. 23(7), 477-479 (1978).
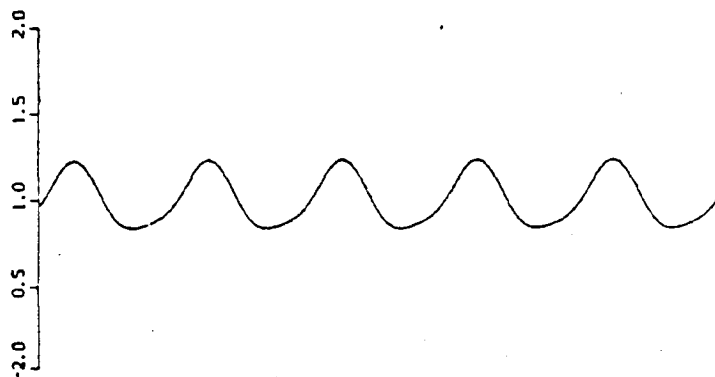
Figure 1
Analytical prediction of flame front speed for ε = 0.3

Figure 2
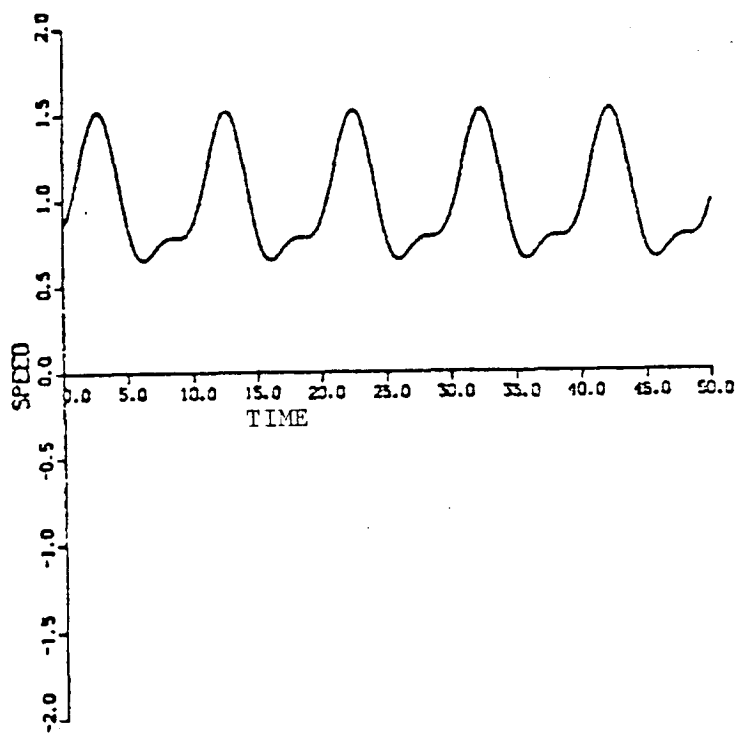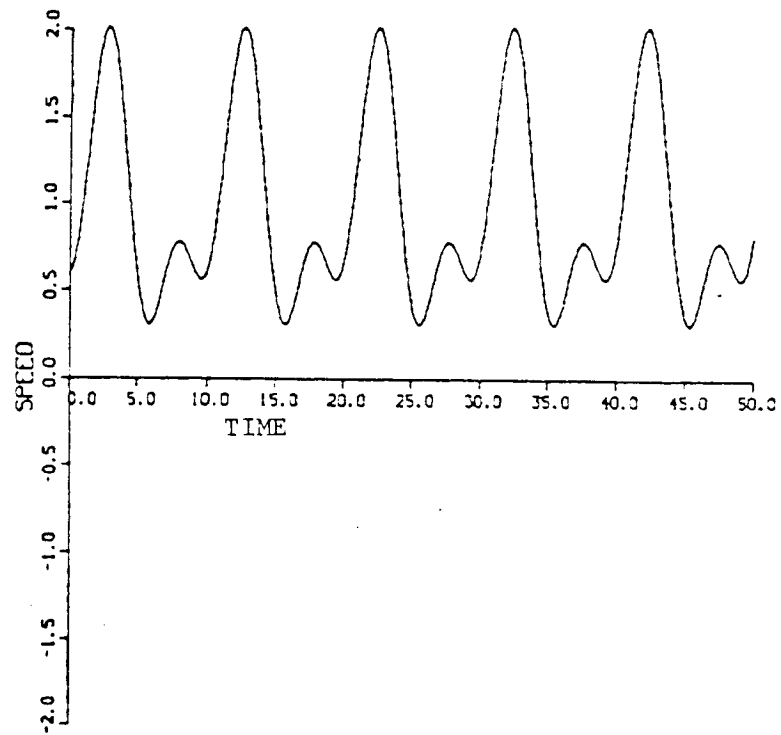Analytical prediction of flame front speed for ε = 0.6

Figure 3
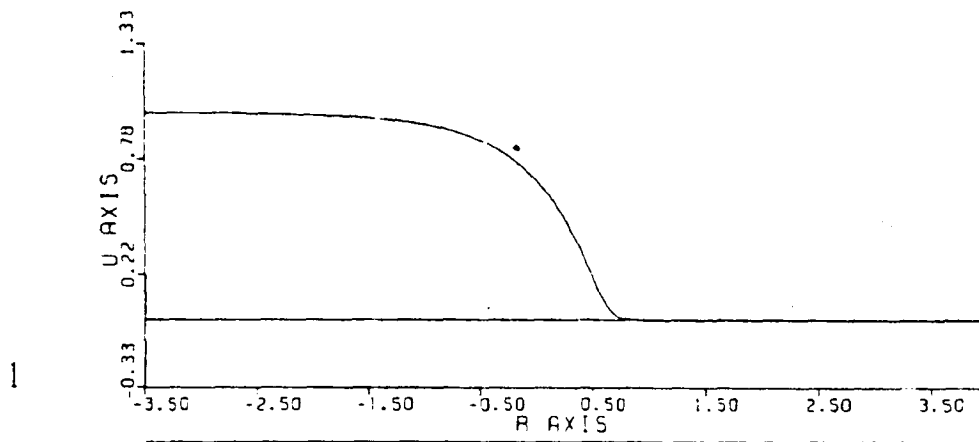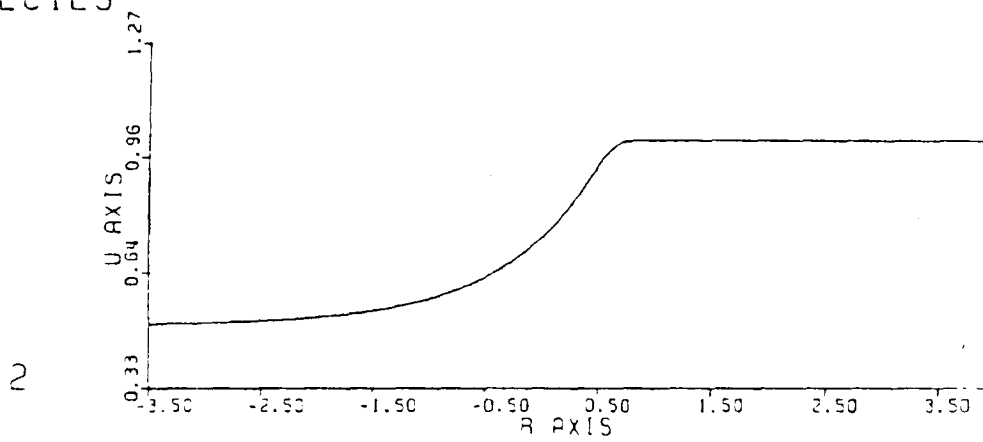Analytical prediction of flame front speed for $\varepsilon = 1.0$
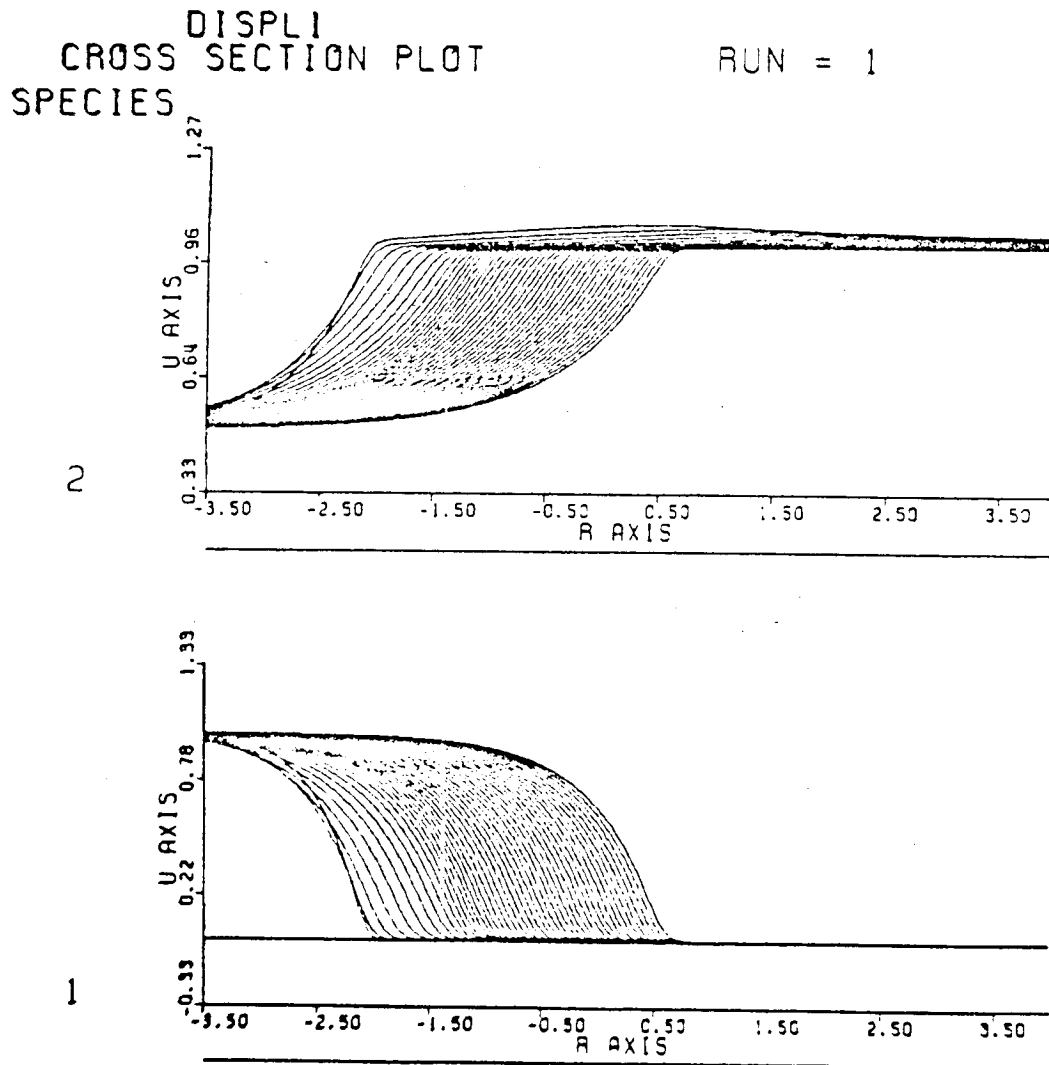
Figure 4
A typical flame profile (L = 1.5)

Figure 5
Superimposed flame profiles for L = 1.5.
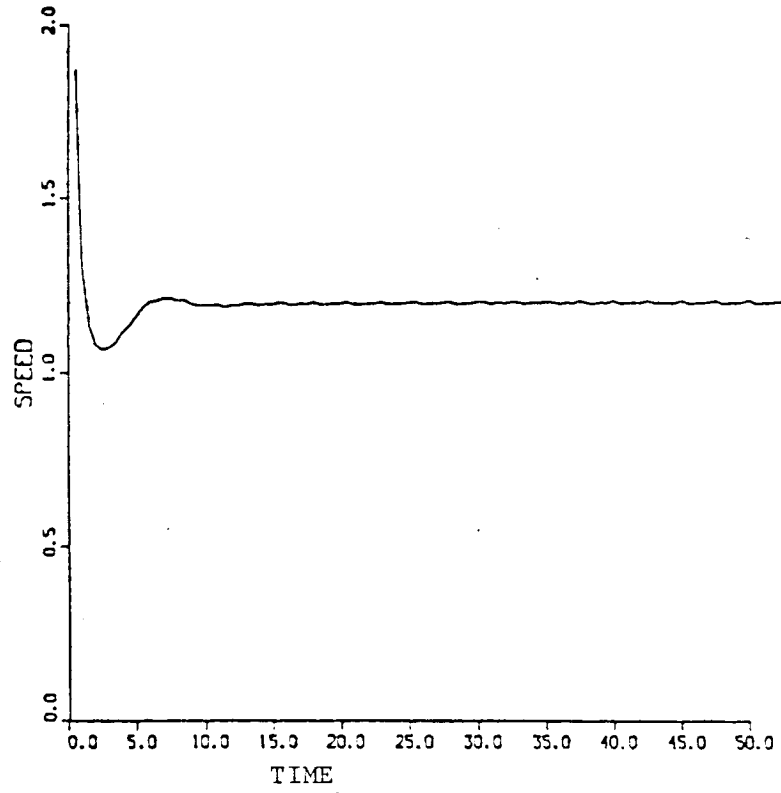The flame is travelling from left to right.
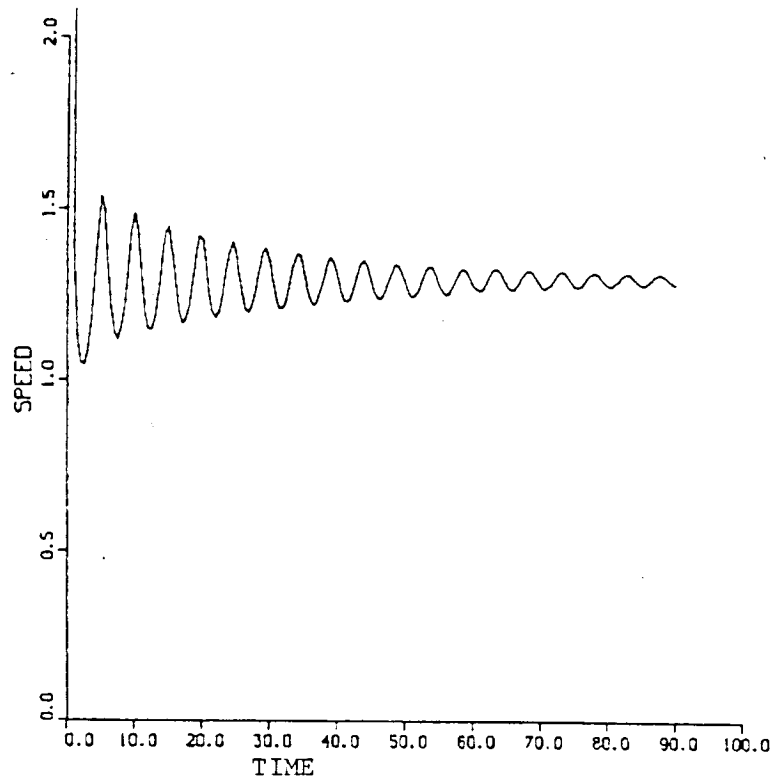
Figure 6
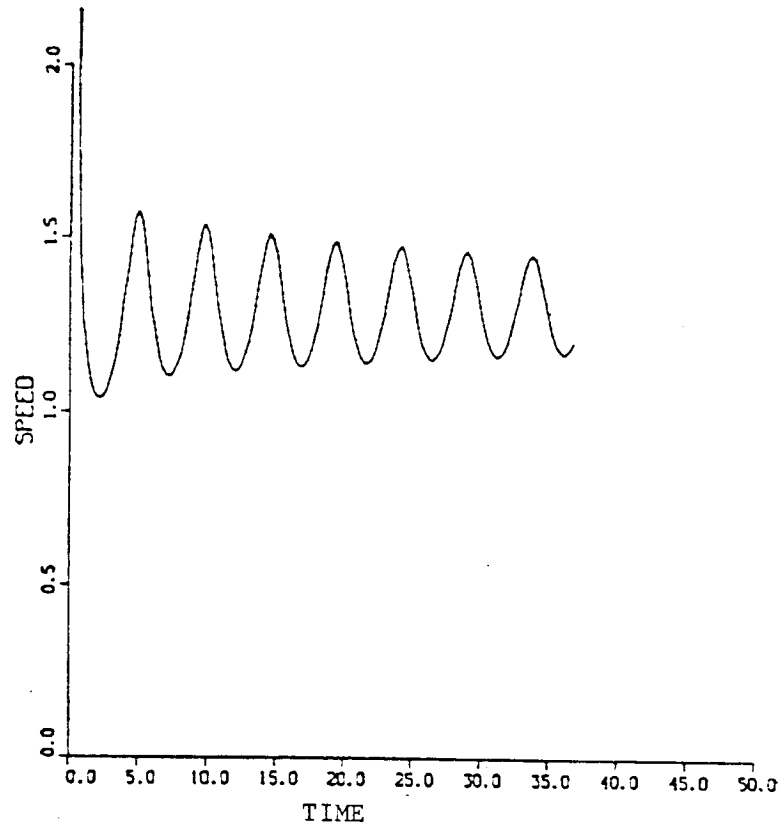Flame front speed (L = 1.5)

Figure 7
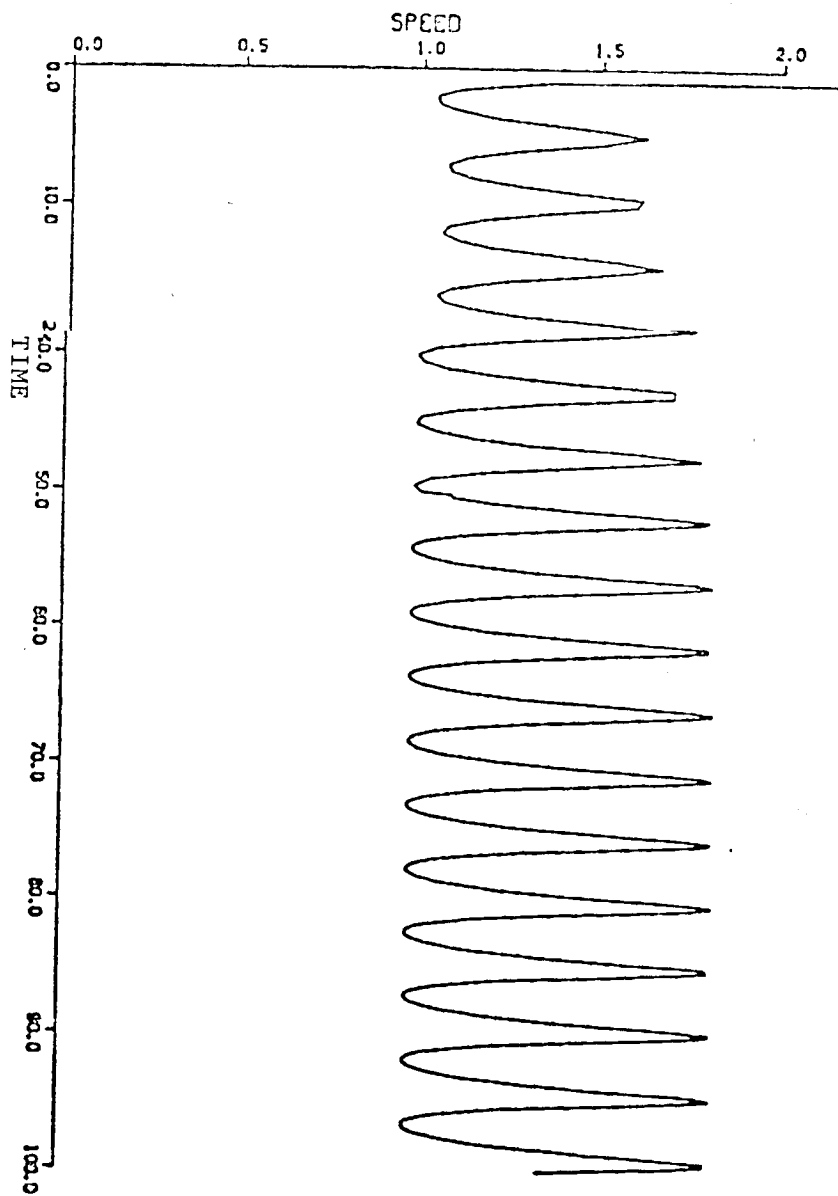Flame front speed (L = 1.8)

Figure 8
Flame front speed (L = 1.81)

Figure 9
Flame front speed (L = 1.83)

Figure 10
Flame front speed (L = 1.85)
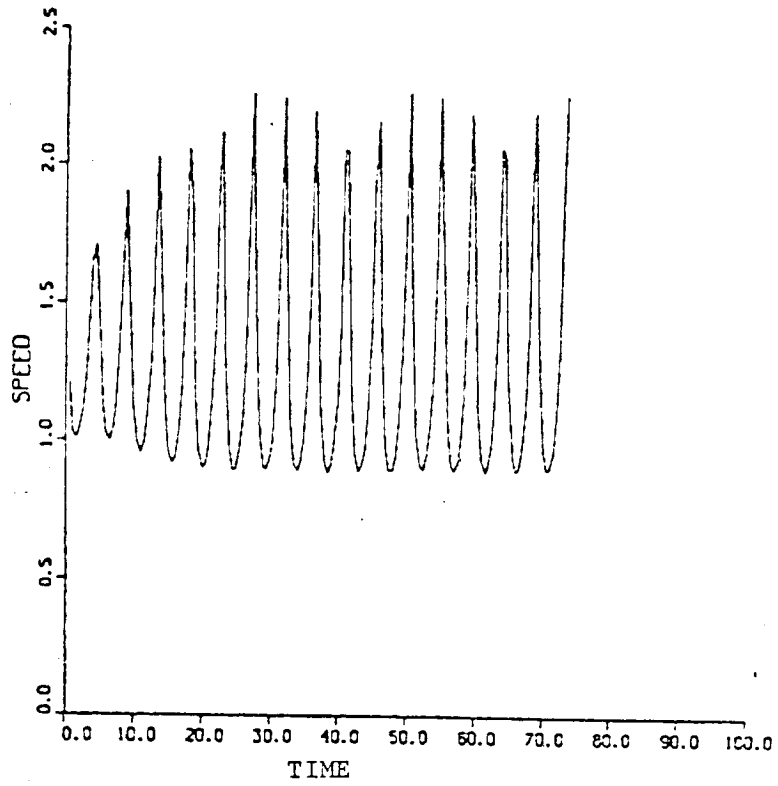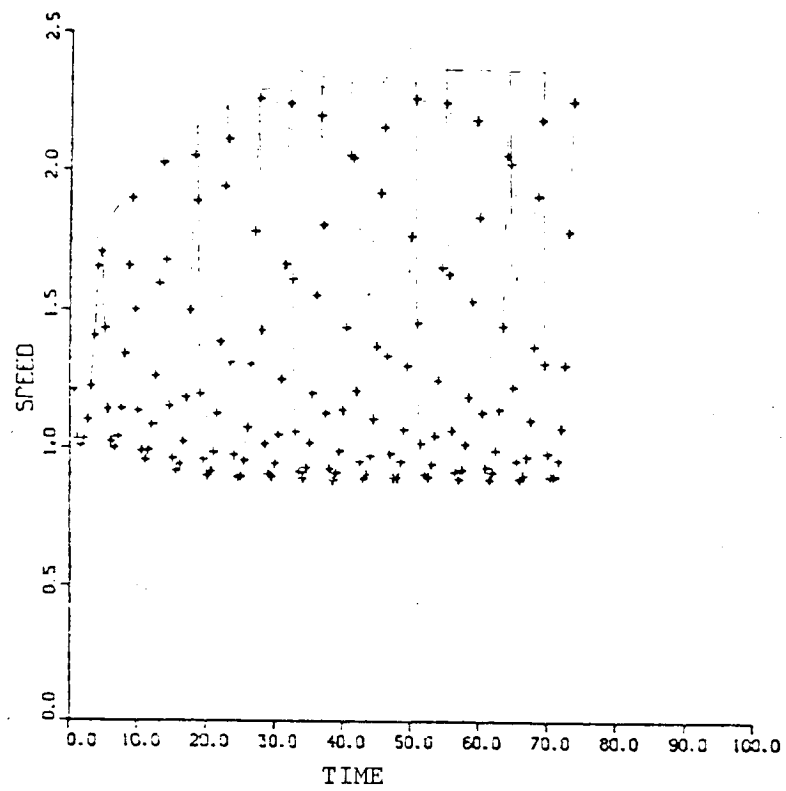
Figure 11
A smooth fit of the flame front speed for L = 1.85

DISPL1
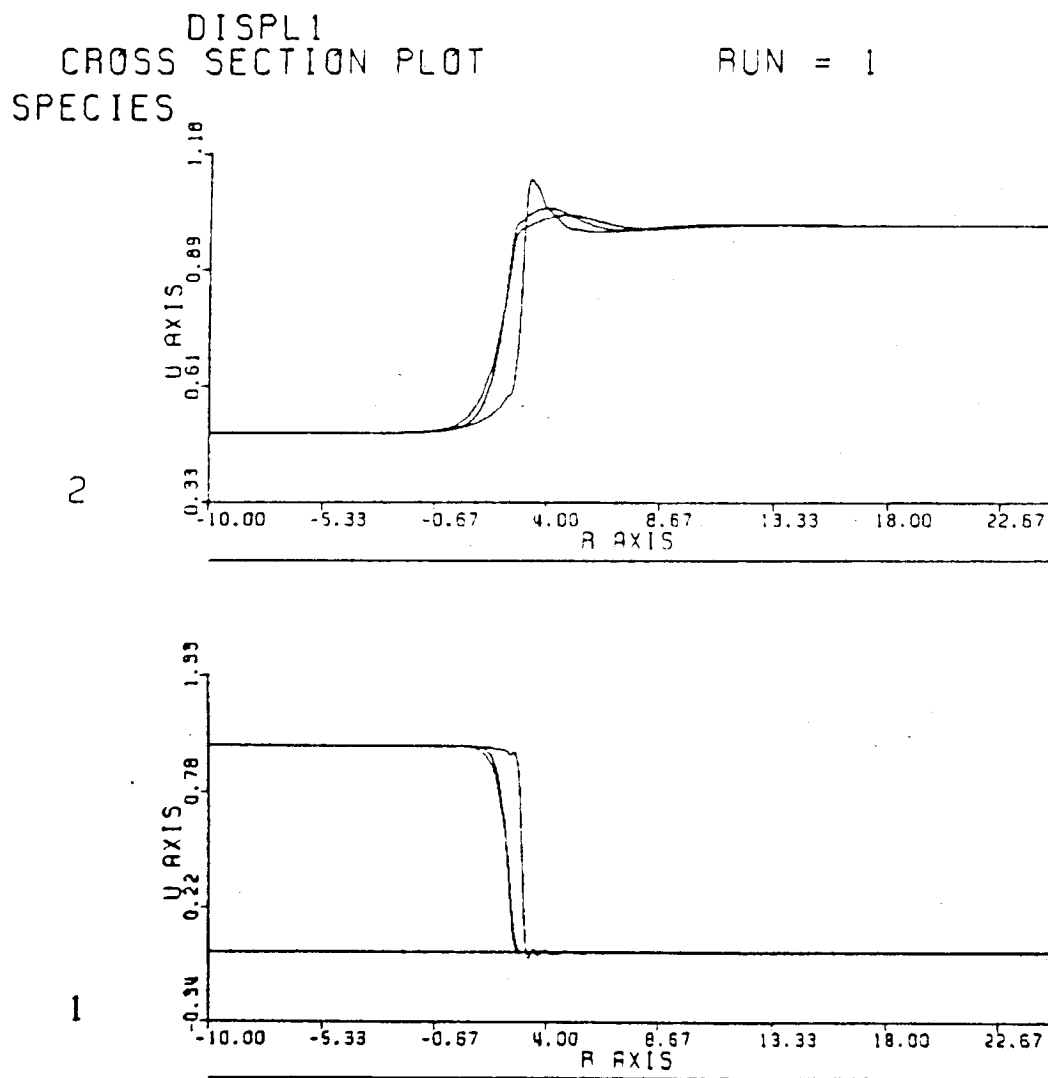CROSS SECTION PLOT   RUN = 1
SPECIES

Figure 12
Successive flame profiles from a course mesh run
with L = 2.1