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FLAT FLAME OLYMPICS: TEST PROBLEM A

Terence P. Coffee

October 1982



US ARMY ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

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Abstract (Cont'd):

20. state problems with elementary chemistry was modified to use the simplified transport and chemistry of the test problem and to follow the details of the transient solution.

The problem is solved for six cases. The cases differ in the Lewis number chosen and the activation energy of the single reaction. The initial conditions used are the steady state solutions predicted by the simplified analytic method of asymptotic analysis.

In most cases, the numerical solutions rapidly converge, and the steady state solutions are similar to the asymptotic solutions. However, in one case, with high activation energy and Lewis number equal to two, the solution does not converge. Instead, large oscillations in the flame speed and the profiles occur.

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I. INTRODUCTION

We are involved in the modeling of one-dimensional, premixed, laminar, steady-state flames.^{1,2} Our purpose is to determine validated sets of elementary chemical reactions for use in predictive combustion models. This involves developing numerical methods to solve premixed flame problems with complex chemistry and transport properties.^{3,4}

This report discusses a test problem for the numerical methods. The problem was proposed by GAMM (Committee for Numerical Methods in Fluid Mechanics), and has been solved for presentation at a workshop at the Technical University, Aachen, Germany, 12-14 Oct 81.

The purpose of the workshop is to bring together the small group of scientists actively working in the field of numerical methods in flame propagation. The workshop will focus on numerical methods that have been developed to solve premixed flame problems. In particular, the meeting will seek to establish the difficulties that result from non-equal diffusivities of heat and matter (Lewis number not equal to one) and the consequences that these have upon the accuracy of the solution.

At the workshop, the solution of two test problems by different numerical schemes will be compared. Here we discuss the first test problem; an unsteady propagating flame with one-step chemistry and Lewis number different from unity. The second test problem, a steady, stoichiometric hydrogen-air flame with complex chemistry, is reported on elsewhere.⁵ The results of the comparisons will be published in the proceedings of the workshop.⁶

¹J.M. Heimerl and T.P. Coffee, "The Detailed Modeling of Premixed, Laminar, Steady-State Flames, I. Ozone," Combustion and Flame, Vol. 39, pp. 301-315, 1980.

²T.P. Coffee and J.M. Heimerl, "Transport Algorithms for Premixed, Laminar, Steady Flames," Combustion and Flame, Vol. 43, pp. 273-289, 1981.

³T.P. Coffee and J.M. Heimerl, "A Method for Computing the Flame Speed for a Laminar, Premixed, One Dimensional Flame," BRL Technical Report, ARBRL-TR-02212, January 1980, (AD-A082803).

⁴T.P. Coffee, "A Computer Code for the Solution of the Equations Governing a Laminar, Premixed, One Dimensional Flame," BRL Memorandum Report, ARBRL-MR-03165, April 1982. (AD A114041)

⁵J.M. Heimerl, "Flat Flame Olympics: Test Problem B," BRL Technical Report, to be published.

⁶Proceedings to be published in Notes on Numerical Fluid Mechanics, Vol. 5, Ed. N. Peters and J. Warnatz, Vieweg-Verlag, publication.

II. THE TEST PROBLEM

The problem is an unsteady propagating flame with one step chemistry (reactant $\rightarrow$ product). The Lewis number may be different from unity. The governing equations are

$$\frac{\partial Y}{\partial t} = \frac{1}{Le} \frac{\partial^2 Y}{\partial x^2} - R \quad (1)$$

and

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + R, \quad (2)$$

where Y is the mass fraction of the reaction, t is the time coordinate, Le is the Lewis number, x is the space coordinate, R is the rate of the reaction, and T is the temperature. All the above quantities are non-dimensional. The reaction rate is given by

$$R = \frac{\beta^2}{2Le} Y \exp \left[-\frac{\beta(1-T)}{1-\alpha(1-T)} \right]. \quad (3)$$

The boundary conditions ($t > 0$) are

$$\begin{aligned} T = 0, Y = 1 \text{ at } x = -\infty \\ \frac{dT}{dx} = \frac{dY}{dx} = 0 \text{ at } x = \infty, \end{aligned} \quad (4)$$

Since we are interested in the transient problem, initial condition must be specified. These are ($t=0$)

$$\begin{aligned} Y = 1 - \exp(Le x) \\ T = \exp(x) \end{aligned} \quad (5)$$

for $x \leq 0$ and

$$Y = 0, t = 1 \quad (6)$$

for $x \geq 0$.

The reaction rate was normalized such that the steady state problem yields the flame velocity -1 in the asymptotic limit $B \rightarrow \infty$. The initial

⁷W.B. Bush and F.E. Fendell, "Asymptotic Analysis of Laminar Flame Propagation for General Lewis Numbers," Combustion Science and Tech., Vol. 1, pp. 421-428, 1970.

conditions are the profiles generated by the asymptotic analysis. For $x \leq 0$, it is assumed that the chemistry term R is negligibly small (convective-diffusive zone). The profiles can then be shown to be exponential functions. At $x = 0$, it is assumed that adiabatic conditions have been achieved. There are discontinuities in the first derivatives at $x = 0$.

The parameter α is taken to be 0.8. There are six cases to be solved; these are given in Table 1. The desired output is the flame velocity, the frequency and amplitude of flame velocity oscillations, if observed, and the enthalpy profile. In the above normalization, the enthalpy H is given by

$$H = Y + T. \quad (7)$$

If the Lewis number is equal to one, we can add Eqs. (1) and (2) and obtain

$$\frac{\partial H}{\partial t} = \frac{\partial^2 H}{\partial x^2} \quad (8)$$

Using the boundary conditions, we can obtain

$$H = Y + T = 1. \quad (9)$$

So the Y equation can be eliminated.

TABLE 1. THE CHOICES OF THE INPUT PARAMETERS TO BE USED

Case	B	L_C
1	10	1.0
2	10	2.0
3	10	0.5
4	20	1.0
5	20	2.0
6	20	0.5

Because of the above simplification, the choice of Lewis number equal to one is a common assumption. One purpose of the problem as given is to observe what effect other choices of the Lewis number may have.

The above problem is somewhat ambiguous in requesting the transient flame velocity. The flame velocity is defined as the speed at which the flame front propagates with respect to the unburned mixture. At steady state, this is well defined. But while approaching steady state, the flame front can change shape, and one part of the flame travel more rapidly than another.

We arbitrarily chose to compute the flame speed with respect to $T = 0.5$. This is the average of the unburned and the adiabatic temperature.

It will be useful to introduce a coordinate transformation

$$\psi = x + x_c(t) \quad (10)$$

$$x_c(0) = 0.$$

Then by the chain rule

$$\frac{\partial Y}{\partial t} + \frac{\partial Y}{\partial \psi} \frac{\partial \psi}{\partial t} = \frac{1}{Le} \frac{\partial^2 Y}{\partial \psi^2} - R \quad (11)$$

and

$$\frac{\partial T}{\partial t} + \frac{\partial T}{\partial \psi} \frac{\partial \psi}{\partial t} = \frac{\partial^2 T}{\partial \psi^2} + R. \quad (12)$$

We will define x_c in such a way that the point $T = 0.5$ remains at the same point in ψ space. From the initial conditions, this means $T = 0.5$ at $\psi = \ln(0.5)$. The details of this procedure are given in the next section.

We will use the notation

$$SP(t) = \frac{\partial \psi}{\partial t} = \frac{\partial x_c}{\partial t}. \quad (13)$$

The equations defining the flame front become

$$\frac{\partial Y}{\partial t} = - SP \frac{\partial Y}{\partial \psi} + \frac{1}{Le} \frac{\partial^2 Y}{\partial \psi^2} - R \quad (14)$$

and

$$\frac{\partial T}{\partial t} = - SP \frac{\partial T}{\partial \psi} + \frac{\partial^2 T}{\partial \psi^2} + R. \quad (15)$$

$SP(t)$ is the speed of the origin of the (ψ, t) coordinate system with respect to the (x, t) coordinate system. Since the flame is in a fixed location in the (ψ, t) system, $SP(t)$ is also the negative of the velocity of the flame (the flame propagates toward $x = -\infty$). As the flame approaches steady state, $SP(t)$ approaches the steady state speed of the flame front, and $\partial T/\partial t$ and $\partial Y/\partial t$ approach zero.

III. THE NUMERICAL SCHEME

The package PDECOL, developed by Madsen and Sincovec, was used to solve the above equations.⁸ This is a general package for solving partial differential equations. It has been modified so as to efficiently solve flame problems.

The spatial discretization is accomplished by finite element collocation methods based on B-splines.⁹ The basic assumption is that the solution can be written in the form

$$Y = \sum_{i=1}^{NC} c_1^{(i)}(t) B_i(\psi) \text{ and}$$

$$T = \sum_{i=1}^{NC} c_2^{(i)}(t) B_i(\psi) , \quad (16)$$

where the basis functions $B_i(\psi)$, $i = 1, \dots, NC$, are B-splines and span the solution space for any fixed t to within a small error tolerance. The time dependent coefficients $c_k^{(i)}$ are determined uniquely by requiring that the expansion above satisfy the given boundary conditions and that they satisfy Eqs. (14) and (15) exactly at $(NC-2)$ interior (collocation) points. The B_i are piecewise polynomials of order KORD. Given a user supplied set of NB breakpoints, (i.e., a set of strictly increasing locations where the polynomials are joined), and the number of continuity equations, NCC, to be applied at the breakpoints, PDECOL generates a set of $NC = KORD (NB-1) - NCC(NB-2)$ basis functions and collocation points. Since by definition a B-spline is zero except over a small interval, at any collocation point no more than KORD of the B-splines are non-zero. So the system of ODE's for the coefficients $c_k^{(i)}$ will not be fully coupled.

Fairly general boundary conditions are allowed. They are also converted into ODE's.

The system of ODE's is integrated in time, using a variant of the Gear stiff implicit integrator. The appropriate banded Jacobian is generated internally by the program.

⁸N.K. Madsen and R.F. Sincovec, "Algorithm 540. PDECOL, General Collocation Software for Partial Differential Equations [D3], *ACMTOMS*, Vol. 5, pp. 326-351, 1979.

⁹C. deBoor, "Package for Calculating with B-Splines," *Siam. J. Numer. Anal.*, Vol. 14, pp. 441-472, 1977.

The time integration is controlled by a user supplied error tolerance ϵ . Single step error estimates divided by $\text{CMAX}_k^{(i)}$ will be kept less than ϵ in the root-mean-square norm. In PDECOL, $\text{CMAX}_k^{(i)}$ is initially set to the maximum of $|c_k^{(i)}|$ and 1.0. Thereafter, $\text{CMAX}_k^{(i)}$ is the largest value of $|c_k^{(i)}|$ seen so far, or the initial $\text{CMAX}_k^{(i)}$ if that is larger. This error criterion is not appropriate for flames. In some locations species concentrations will approach zero, and we do not want to waste time computing a negligible concentration very accurately.

So we introduce a semi-relative error control. $\text{CMAX}_k^{(i)}$ will be chosen as the maximum of $c_k^{(i)}$ and a user supplied parameter SREC. So mass fractions less than SREC will be computed less accurately. In this paper, $\text{SREC} = 10^{-3}$.

The original program PDECOL is fully implicit. That is, the Jacobian of the set of ODE's is used to advance the time integration.¹⁰

Our main interest is in the steady state solution of flames with detailed chemistry. Such flames involve relatively large numbers of chemical species and hence PDE's. As the number of PDE's increase, both the overall dimensions of the Jacobian and the bandwidth increase rapidly. This creates problems both in terms of storage space and execution time.

So we essentially uncouple the equations and solve them successively. We assume that changes in one PDE do not effect the others. That is, the terms in the Jacobian relating to the effect of one PDE on another are set equal to zero. Then the Jacobian matrix can be decomposed into smaller matrices, one for each PDE.

To integrate a time step, the predictor of the predictor-corrector method is used to get first estimates for all the $c_k^{(i)}$ at the new time. Then we solve for the $c_1^{(i)}$, using the first small Jacobian, and assuming that the other $c_k^{(i)}$ do not change. Then we use the new values for $c_1^{(i)}$, the predicted values for $c_k^{(i)}$, $k > 2$, and solve for $c_2^{(i)}$. This continues for all the PDE's. The error is estimated, and, if necessary, the above procedure is iterated.

This procedure is similar to one developed by Spalding and Stephenson for use in a finite difference code.¹¹

For the present problem, there are only two PDE's. Moreover, the details of the transient solution are required. In this case it would be more efficient to use the full Jacobian. However, we did not want to rewrite the code, so it was run using successive calculation. As a result, smaller time steps probable had to be taken to obtain the same accuracy.

¹⁰A.C. Hindmarsh, "Preliminary Documentation of GEARIB. Solution of Implicit Systems of Ordinary Differential Equations with Banded Jacobian," Rep. UCID-30130, Lawrence Livermore Laboratory, 1976.

¹¹D.B. Spalding and P.L. Stephenson, "Laminar Flame Propagation in Hydrogen + Bromide Mixtures, Proc. R. Soc. Lond. A, Vol. 324, pp. 315-337, 1971.

The flame front will be kept near the center of the interval of integration, so the breakpoints should be densest here. Rather than choosing the breakpoint sequence by hand, an algorithm has been written to generate an appropriate set of breakpoints.

The user supplies L, the total length of the interval of integration; NINT, the total number of subintervals (NB=NINT+1); NCN, the number of subintervals of equal length that will be at the center of the interval of integration; and FC, the ratio between the longest subintervals (on the boundaries) and the shortest subintervals.

The program generates a set of subintervals whose lengths increase by a constant factor γ , where

$$\gamma = \log^{-1} (2(\log FC)/(NINT-NCN)). \quad (17)$$

The common length LC of the NCN shortest subintervals in the center is

$$LC = L / (NCN + 2\gamma(\gamma^{(NINT-NCN)/2} - 1) / (\gamma - 1)). \quad (18)$$

To actually run the code for the transient problem, the user chooses the defining parameters α, β , and L_e . Then the numerical parameters L, NINT, NCN, FC, KORD, NCC, and TFINAL must be chosen. TFINAL is the time t the code will integrate to. In this paper we always choose KORD=4 and NCC = 2 (cubic splines).

The boundary values ψ_L and ψ_R are chosen as approximately $-L/2$ and $L/2$. These are adjusted slightly so the value $\ln(.5)$ is a collocation point. So the value $T = 0.5$ is at a point where the computation is most accurate.

As the time integration proceeds, we require that $\partial T / \partial t$ equal zero at this collocation point. This is done by adjusting the value of SP. At $t = 0$, we choose $SP(t) = 0$, then integrate one time step. At the end of the time step, evaluate $\partial T / \partial t$ and $\partial T / \partial \psi$, using the expansion (16) and the space derivative of the expansion.

Now choose

$$SPF = (\partial T / \partial t) / (\partial T / \partial \psi). \quad (19)$$

If SP was given this value at $t = 0$, the present time derivative would be zero. SPF is taken as the flame speed at the present time. At later time steps increments to SPF are computed in the same fashion.

The flame speed is then computed with a lag of one time step. It is possible for the lag to cause the value $T = 0.5$ to drift away from a fixed location.

So a heuristic correction factor is used. We define

$$FVD = 10(.5 - T) / TFINAL \quad (20)$$

and let

$$SP = (\partial T / \partial t - FVD) / (\partial T / \partial \psi). \quad (21)$$

This value is actually used in the equations.

Even with a moderate error control ($\epsilon = 10^{-3}$) SPF and SP agree to 3 or 4 places. So the drift of the value $T = 0.5$ due to the lag in computing SP has a negligible effect.

This procedure can be checked at steady state ($\partial Y / \partial t = \partial T / \partial t = 0$). Integrating Eq. (14), one obtains

$$SP (Y|_{\psi_R} - Y|_{\psi_L}) = \frac{1}{Le} \left(\frac{\partial Y}{\partial \psi} \Big|_{\psi_R} - \frac{\partial Y}{\partial \psi} \Big|_{\psi_L} - \int_{\psi_L}^{\psi_R} R d\psi \right), \quad (22)$$

The integral is evaluated using the trapezoid rule. At steady state, the value obtained by this procedure should be the same as the value computed from the T equation.

IV. NUMERICAL SOLUTIONS

The test problems were solved using a Cyber 76. The input parameters used are given in Table 2. Table 3 gives the run times, the number of time steps taken, and the steady state flame speeds. The speeds are close to the asymptotic limit of 1. As expected, they are closer to 1 for $B = 20$ than for $B = 10$.

Numerical errors can be introduced because of inadequate spatial resolution (NINT, NCN, and FC) or inadequate temporal resolution (ϵ). Errors can also occur if L is assigned a value that is too small. The profiles may then have nontrivial space derivatives at the boundaries. The boundary conditions will then distort the flame front.

As a check on the numerical accuracy, the problems were rerun with NINT decreased by 25%, ϵ increased by a factor of 3, and L decreased by 10%. The results were virtually identical to those reported here.

Figure 1 shows the flame speed profile for Case 1. The profile is only shown up to $t = 0.5$. After this time there is just a slow approach to the final steady-state value.

TABLE 2. THE COMPUTATIONAL INPUT PARAMETERS FOR THE TEST PROBLEMS

Case	NINT	ϵ	L	NCN	FC	TFINAL
1	40	10^{-4}	20	20	10	10
2	40	10^{-4}	20	20	10	50
3	60	10^{-4}	40	30	30	100
4	40	10^{-4}	20	20	20	10
5	80	10^{-4}	24	40	40	100
6	60	10^{-4}	40	30	40	50

TABLE 3. RESULTS FOR THE TEST PROBLEMS

Case	Run Time	No. of Steps	SP
1	24.1	568	.918
2	18.5	500	.849
3	60.0	898	.958
4	18.7	478	.954
5	404.5	6597	
6	63.7	898	.978

Figure 2 shows the temperature profile for Case 1 for selected values of t . At $t = 0$ there is a slight Gibbs overshoot at $x = 0$ where the exponential function is joined to the straight line. The steep gradient near $x = 0$ causes an increase in the flame speed due to thermal conductivity. This steep gradient relaxes rapidly. There, there is a relatively slow approach to the steady state solution. This is quite close to the asymptotic solution except near $x = 0$.

For Case 1 ($Le = 1$), $Y = 1 - T$ and $H = 1$, so these profiles are not shown.

For Case 2 ($Le = 2$), after the initial flame speed increase the speed drops off rapidly (Figure 3). It then takes a relatively long time to approach steady state (Figure 4).

This occurs because the diffusion of the reactant is now slow. After the initial burst in the flame speed the reactant becomes used up near $x = 0$ and the flame front has not yet moved very far. So the temperature in the flame front decreases. Finally, the flame propagates forward, more Y becomes available, and the temperature profile increases to steady state (Figures 5 and 6). The enthalpy profile (Figure 7) behaves similarly. This kind of overshoot can only occur because the Lewis number is different from unity.

For Case 3, the flame speed profile (figure 8) is similar to Case 1. Diffusion is now faster than thermal conductivity, and there is no overshoot due to lack of reactant.

It is necessary to increase L , the length of the interval of integration. Since diffusion is more rapid, the Y profile is more spread out. Figure 9 shows the Y profile over the same interval as for Case 2. However, the numerical interval must extend further to resolve the approach to the cold boundary condition $Y = 1$. Here we also increase FC , the ratio between the center and boundary subintervals, so that the flame front is still adequately resolved.

Figure 10 shows the T profile, which is not as spread out. The enthalpy profile is given by Figure 11.

The next three cases ($\beta = 20$) have a higher activation energy, so the asymptotic analysis should be more accurate. This is true for Case 4 ($Le = 1$). The flame speed profile shows only a small excursion before reaching steady state (Figure 12). The final T profile (Figure 13) is almost identical to the asymptotic solution.

For case 5 ($Le = 2$) the flame speed profile begins similarly to Case 2 (Figure 14). However, the flame velocity then oscillates (Figure 15) with a period of about 9 time units.

This effect is due to the slowness of the diffusion of Y combined with the high activation energy of R . The Y and T profiles first spread out due to diffusion and thermal conductivity. Then the reaction cuts in. Due to the rapidity of the reaction, a bump occurs in the T profile. In this high temperature region, the supply of Y is exhausted. So the temperature profile again relaxes (Figures 16 and 17) and the profiles oscillate around the

asymptotic solution but do not converge to it. The enthalpy profile (figure 18) behaves similarly.

The last case again converges. The Y profile is spread out by diffusion, but the numerical solution is again very similar to the asymptotic solution.

V. CONCLUSIONS

The results show that for one step chemistry and high activation energy the asymptotic analysis is very accurate. Since the asymptotic analysis does not resolve the flame front, the steep gradient does cause a transient increase in the flame speed before the steady state solution is achieved.

If $Le < 1$, no additional problems occur, except that convergence is somewhat slower. However, the combination of $Le > 1$ and a high activation energy can cause overshoot or even large oscillations.

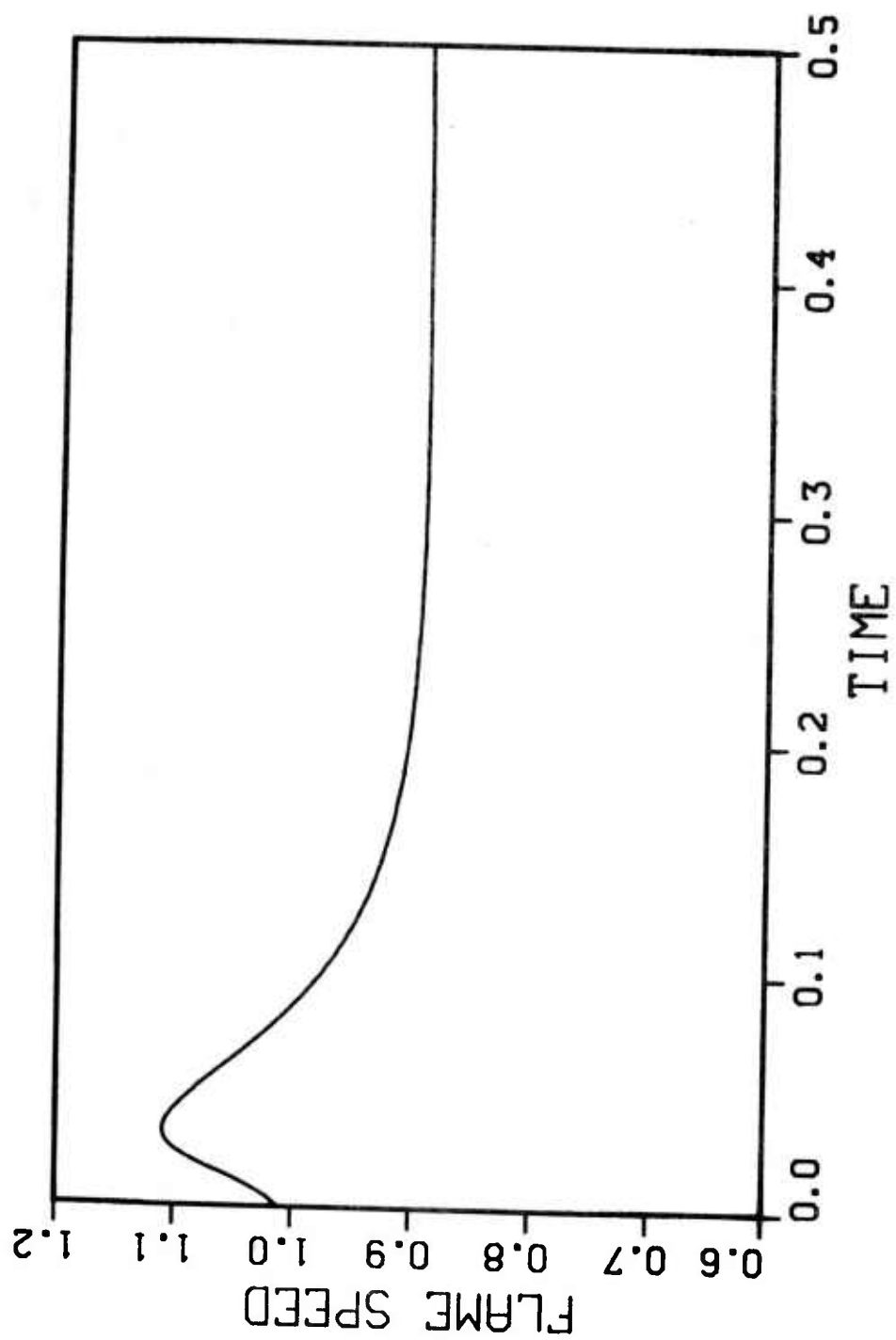


Figure 1. Case 1. Flame Speed Profile.

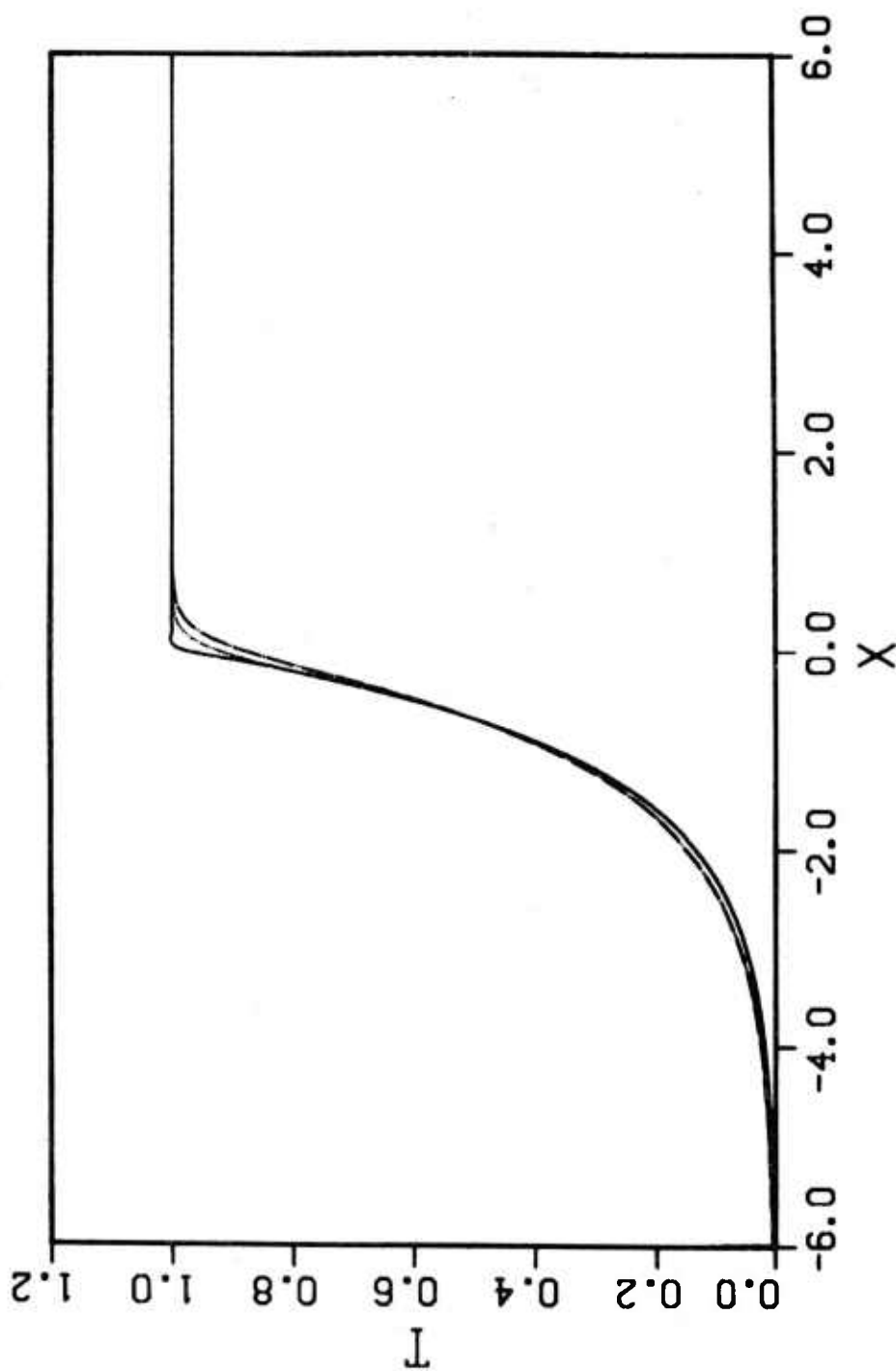


Figure 2. Case 1. Temperature Profile. Time = 0 (line). Time = 0.032 (dot). Time = 10 (chain-dot).

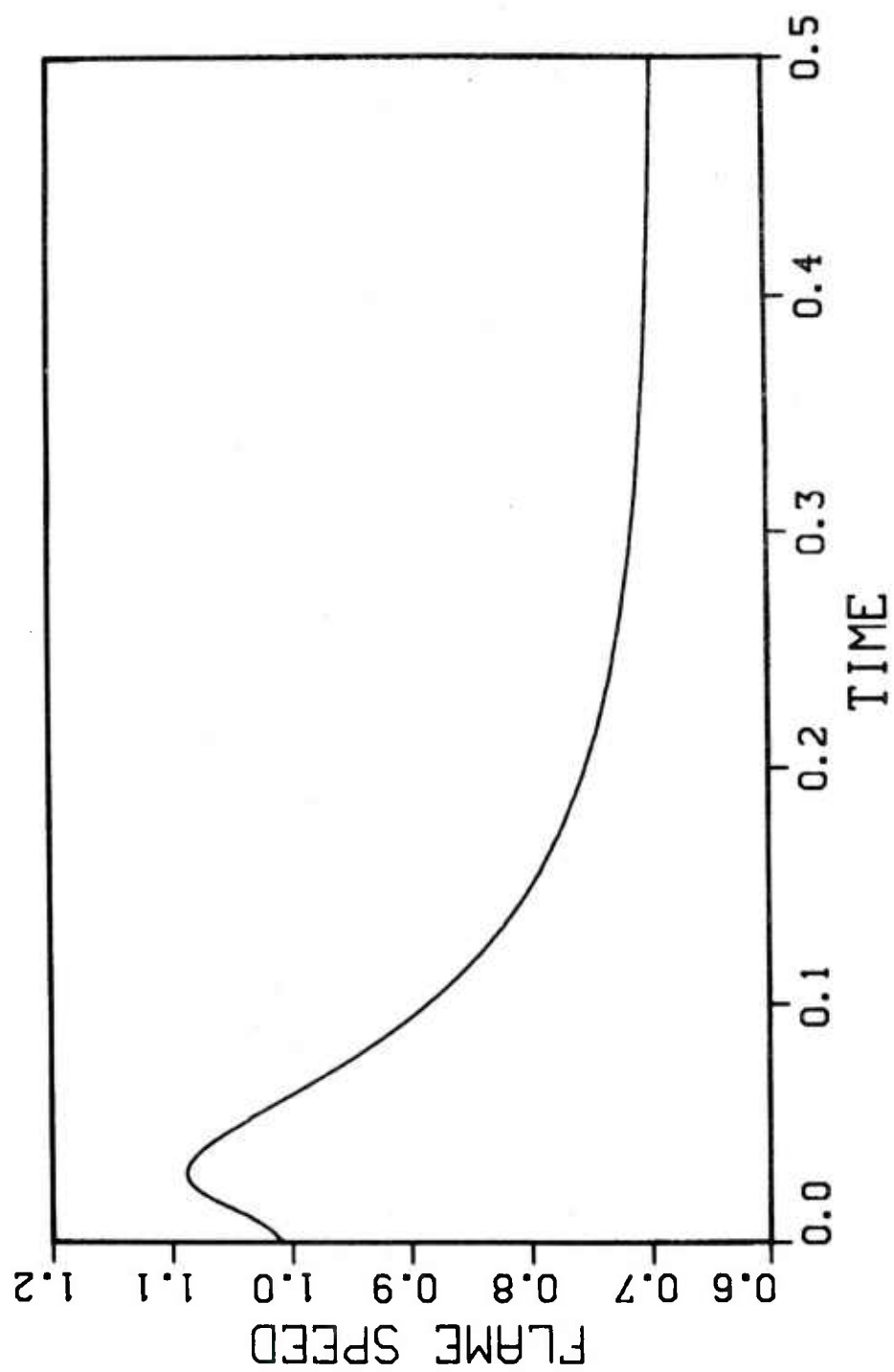


Figure 3. Case 2. Flame Speed Profile ($0 < \text{time} < 0.5$).

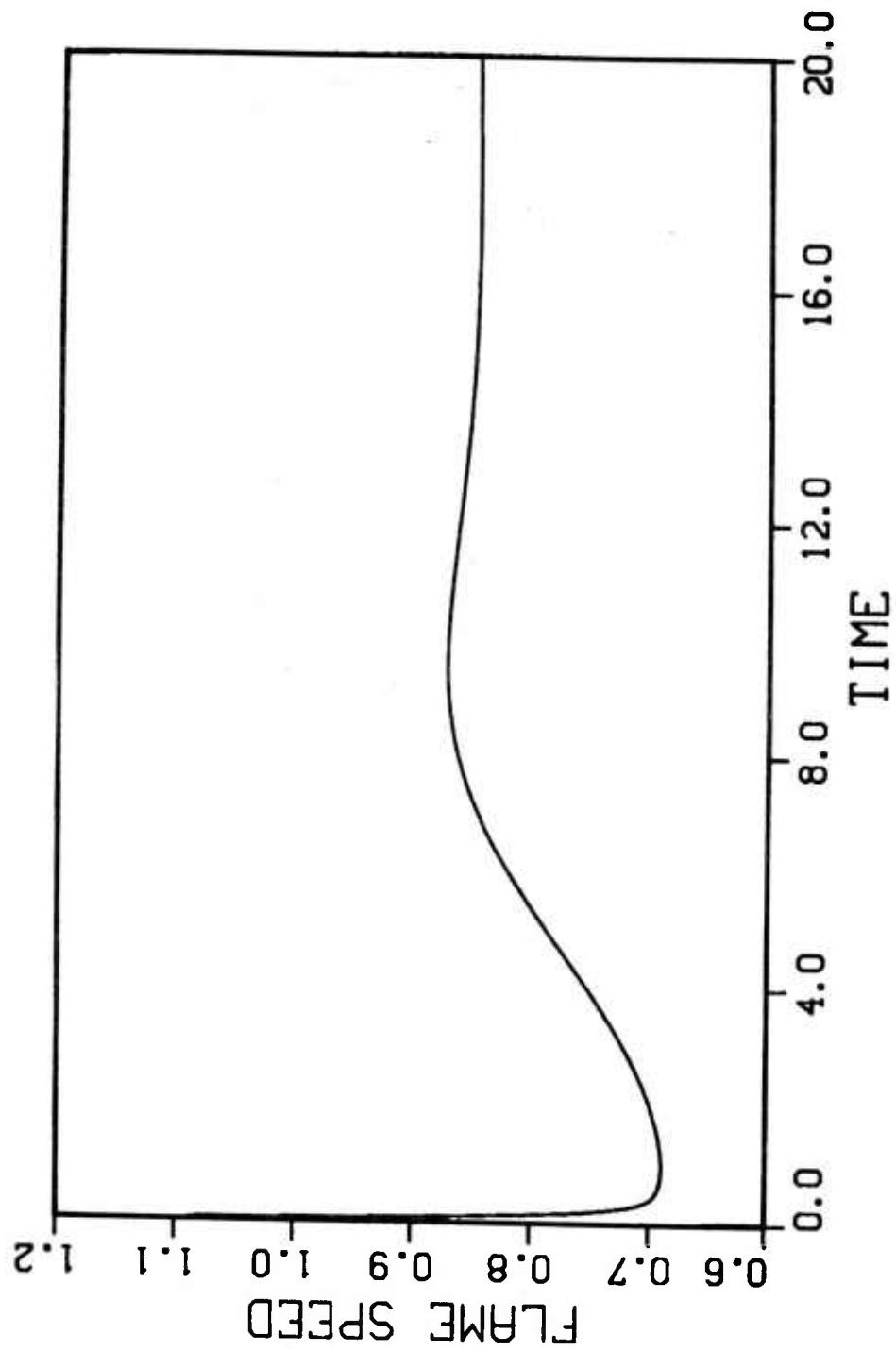


Figure 4. Case 2. Flame Speed Profile ($0 < \text{time} < 20$).

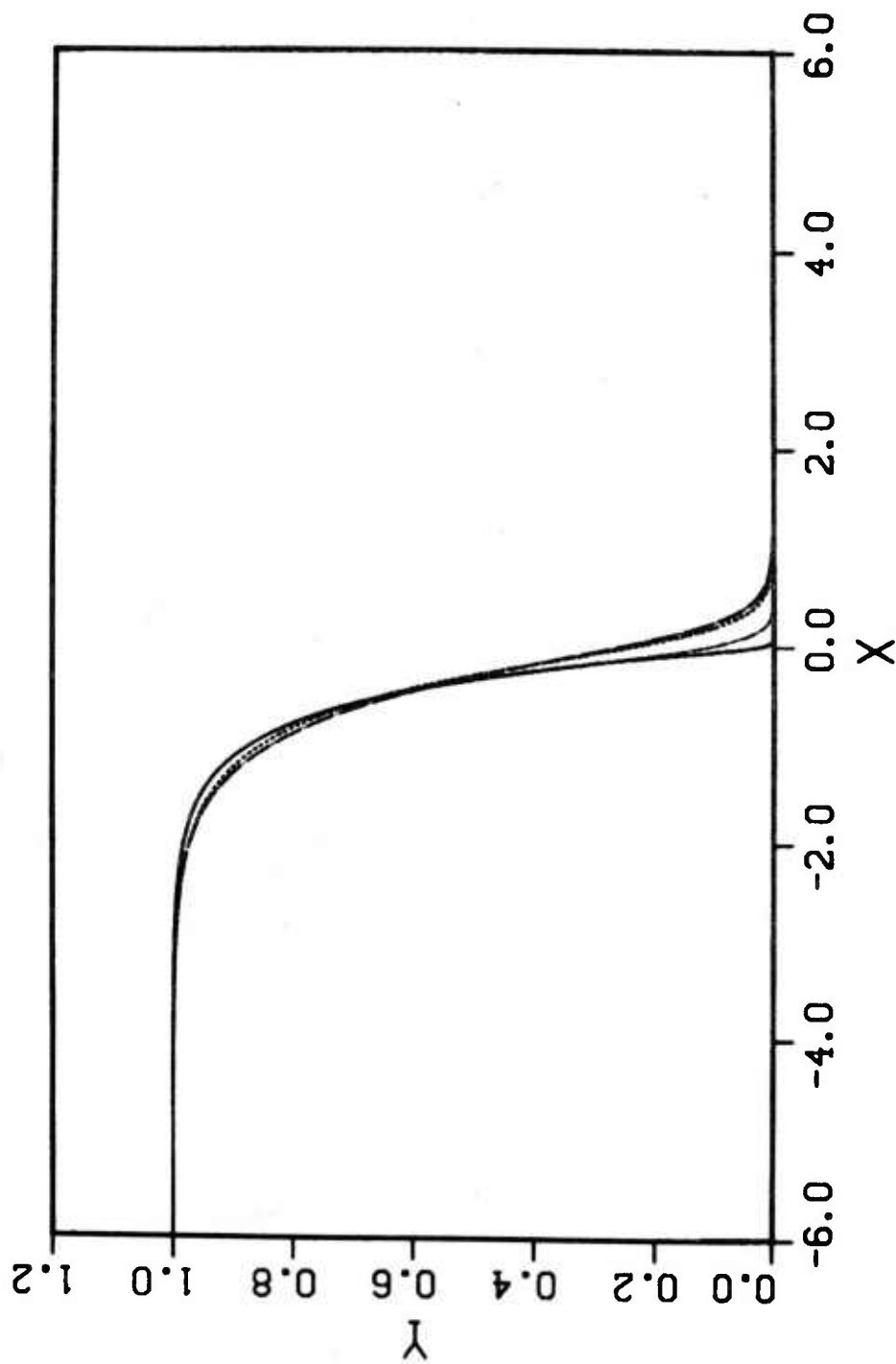


Figure 5. Case 2. Reactant Profile. Time = 0 (line). Time = 0.029 (dot). Time = 0.995 (chain-dot). Time = 50 (dash).

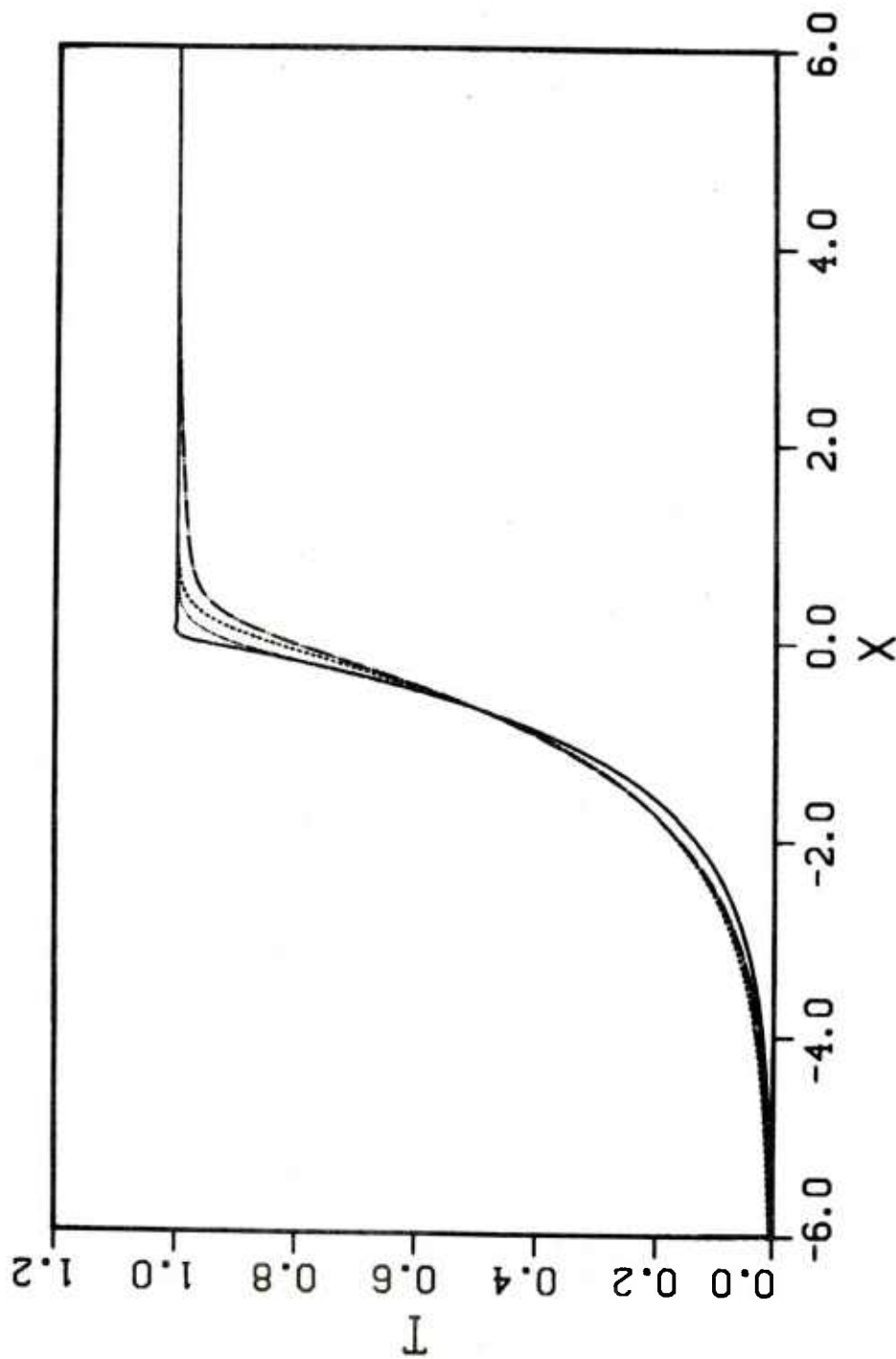


Figure 6. Case 2. Temperature Profile. Time = 0 (line). Time = 0.029 (dot). Time = 0.995 (chain-dot). Time = 50 (dash).

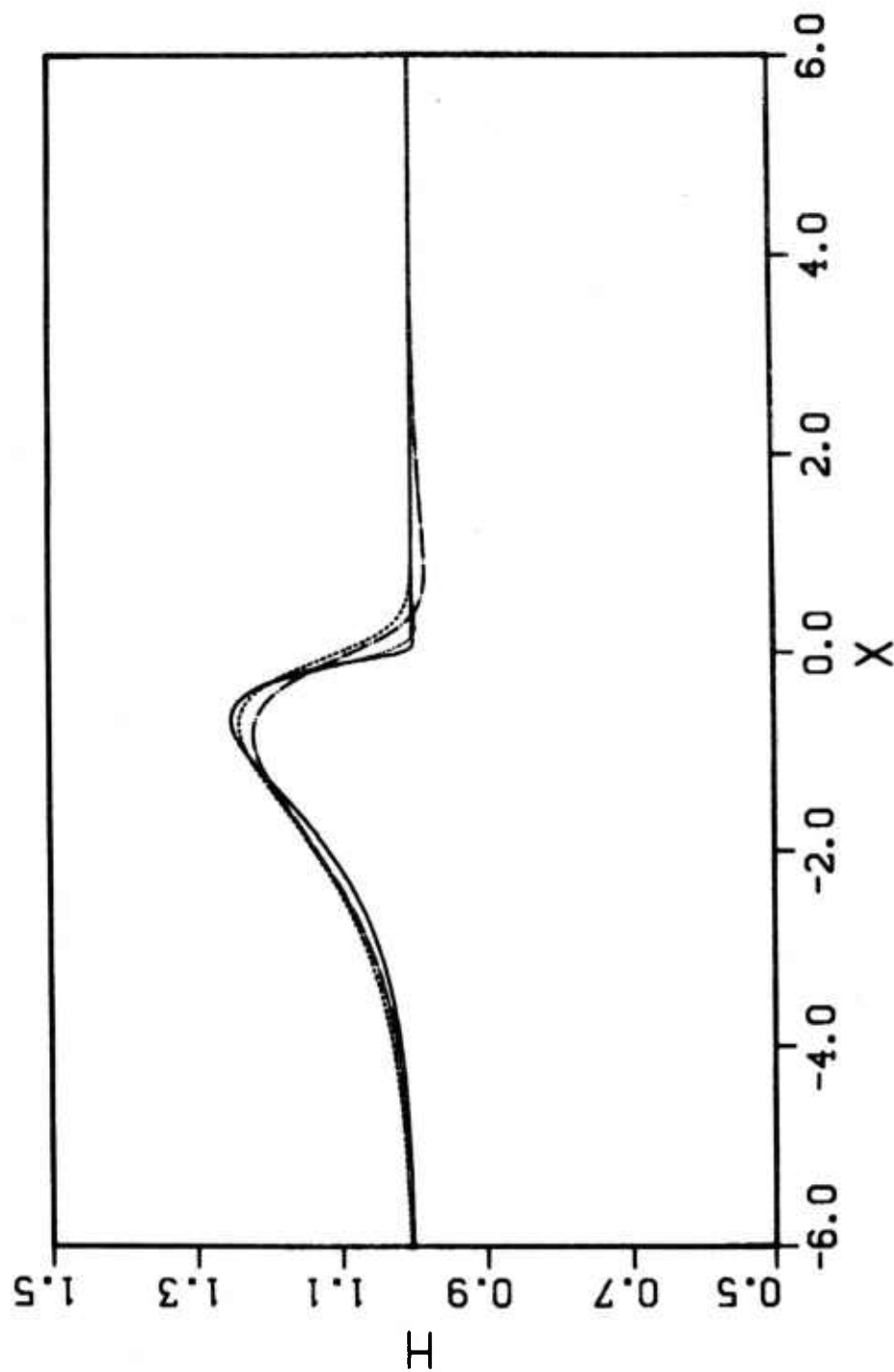


Figure 7. Case 2. Enthalpy Profile. Time = 0 (line). Time = 0.029 (dot). Time = 0.995 (chain-dot). Time = 50 (dash).

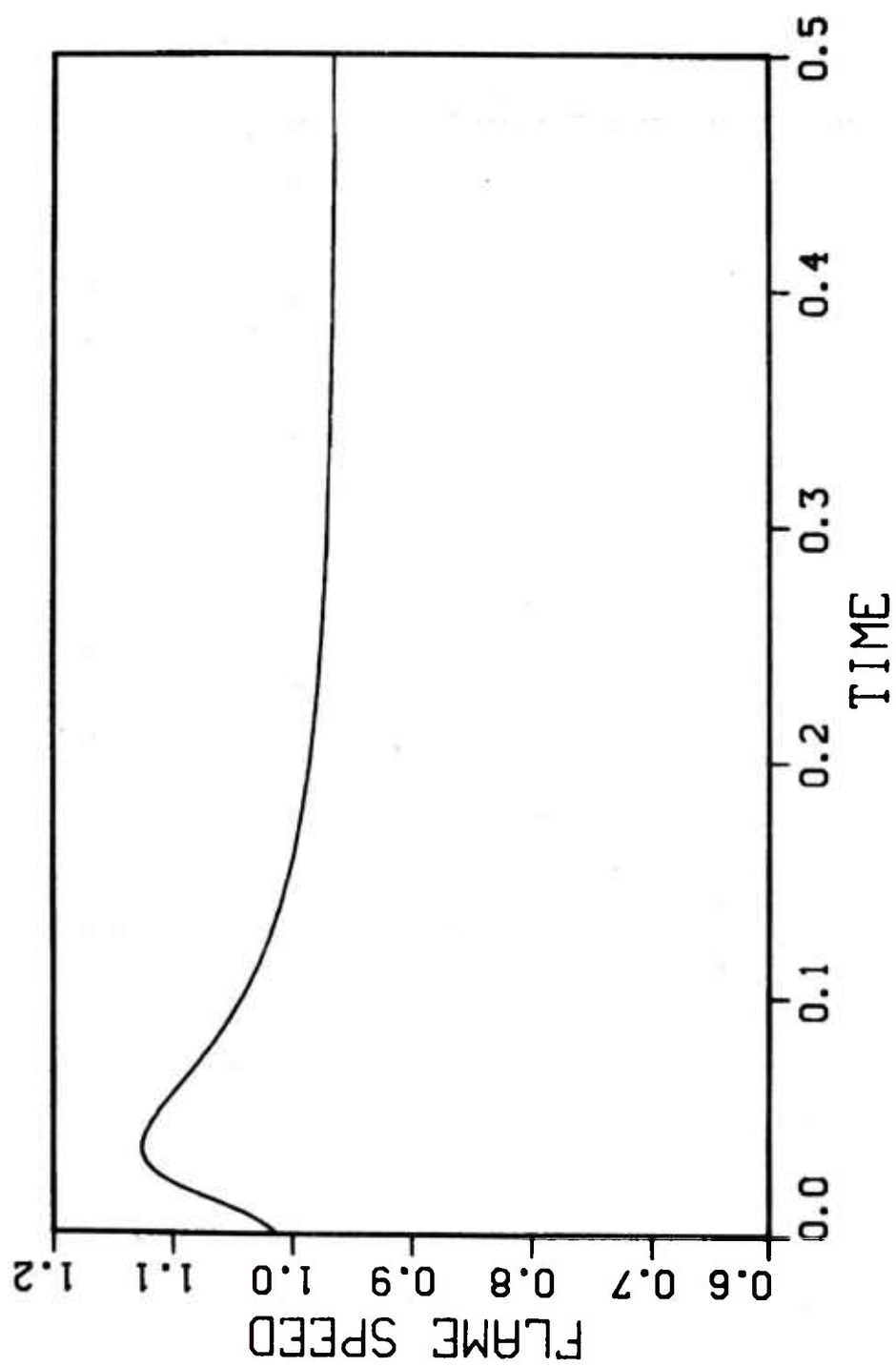


Figure 8. Case 3. Flame Speed Profile.

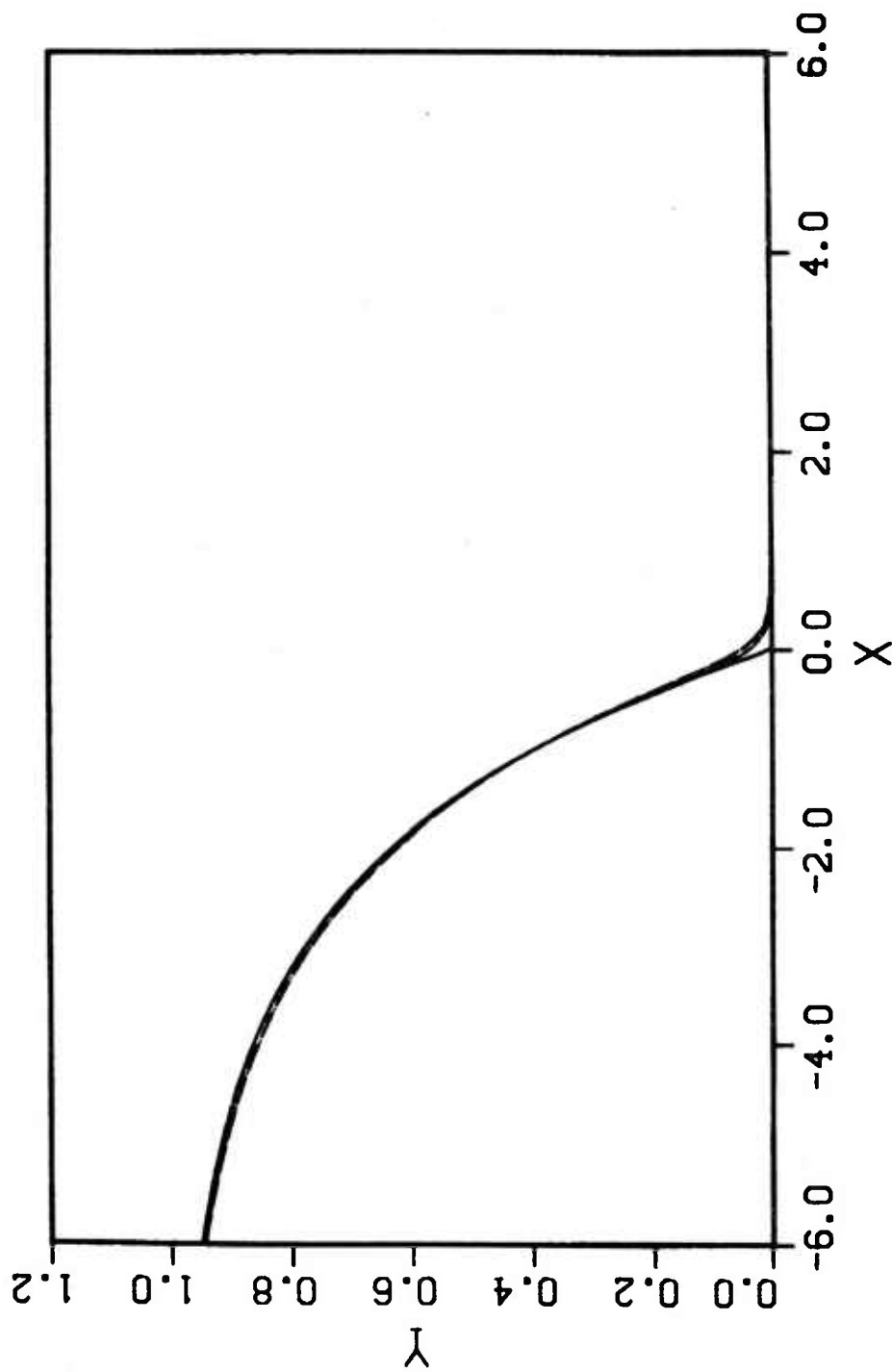


Figure 9. Case 3. Reactant Profile. Time = 0 (line). Time = 0.042 (dot). Time = 50 (chain-dot).

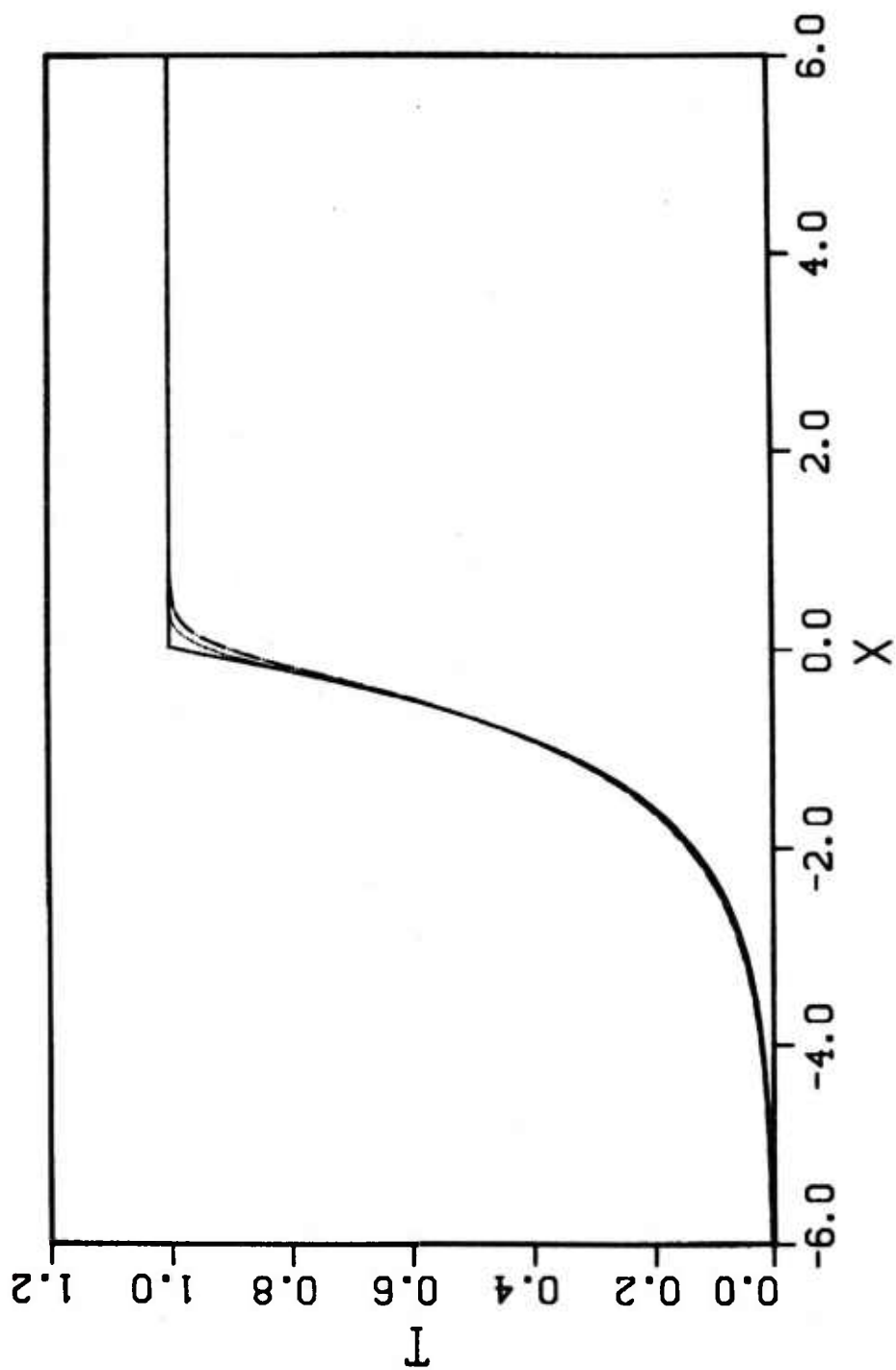


Figure 10. Case 3. Temperature Profile. Time = 0 (line). Time = 50 (chain-dot).

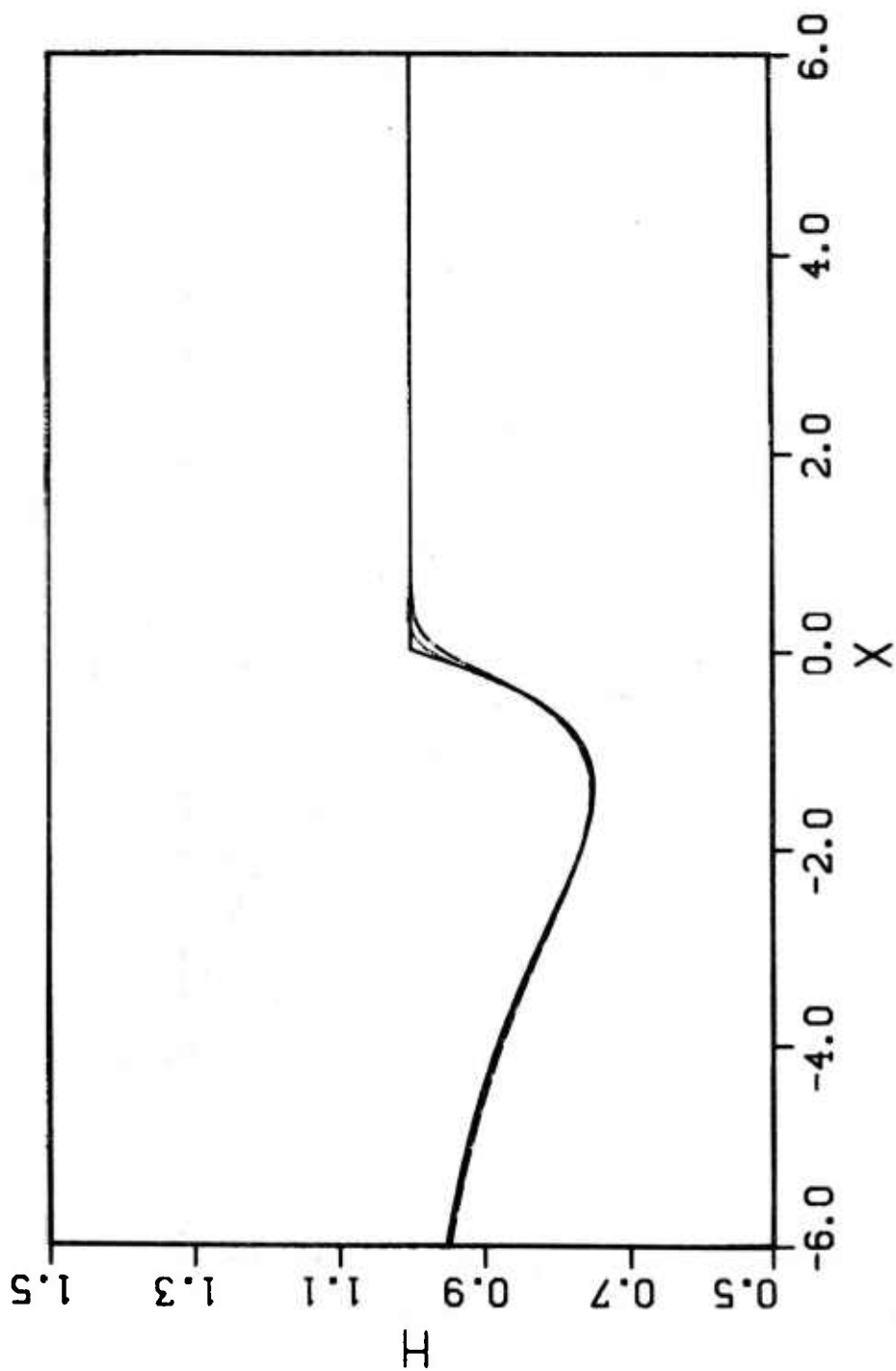


Figure 11. Case 3. Enthalpy Profile. Time = 0 (line). Time = 0.042 (dot). Time = 50 (chain-dot).

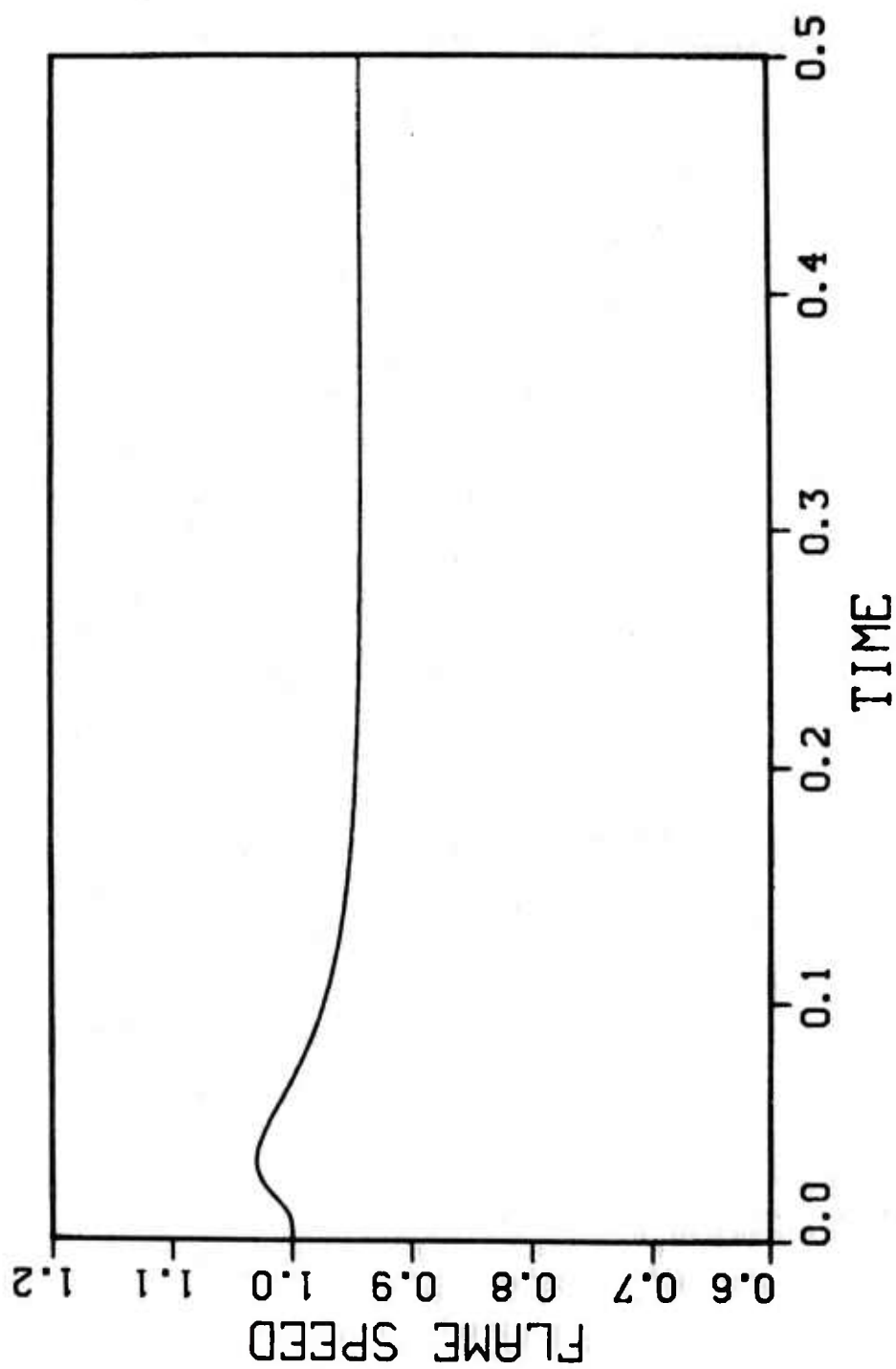


Figure 12. Case 4. Flame Speed Profile.

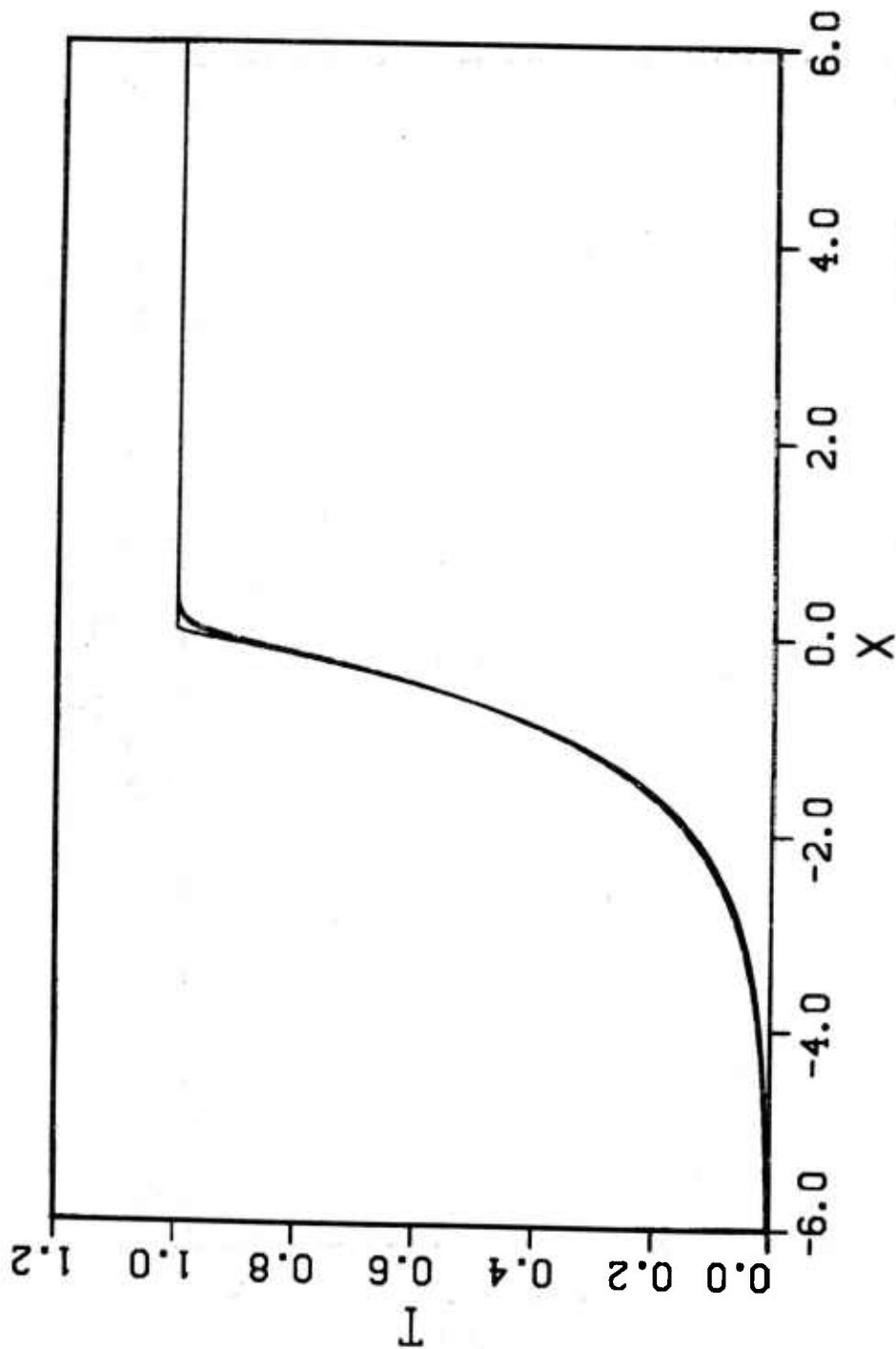


Figure 13. Case 4. Temperature Profile. Time = 0 (line). Time = 0.034 (dot). Time = 10 (chain-dot).

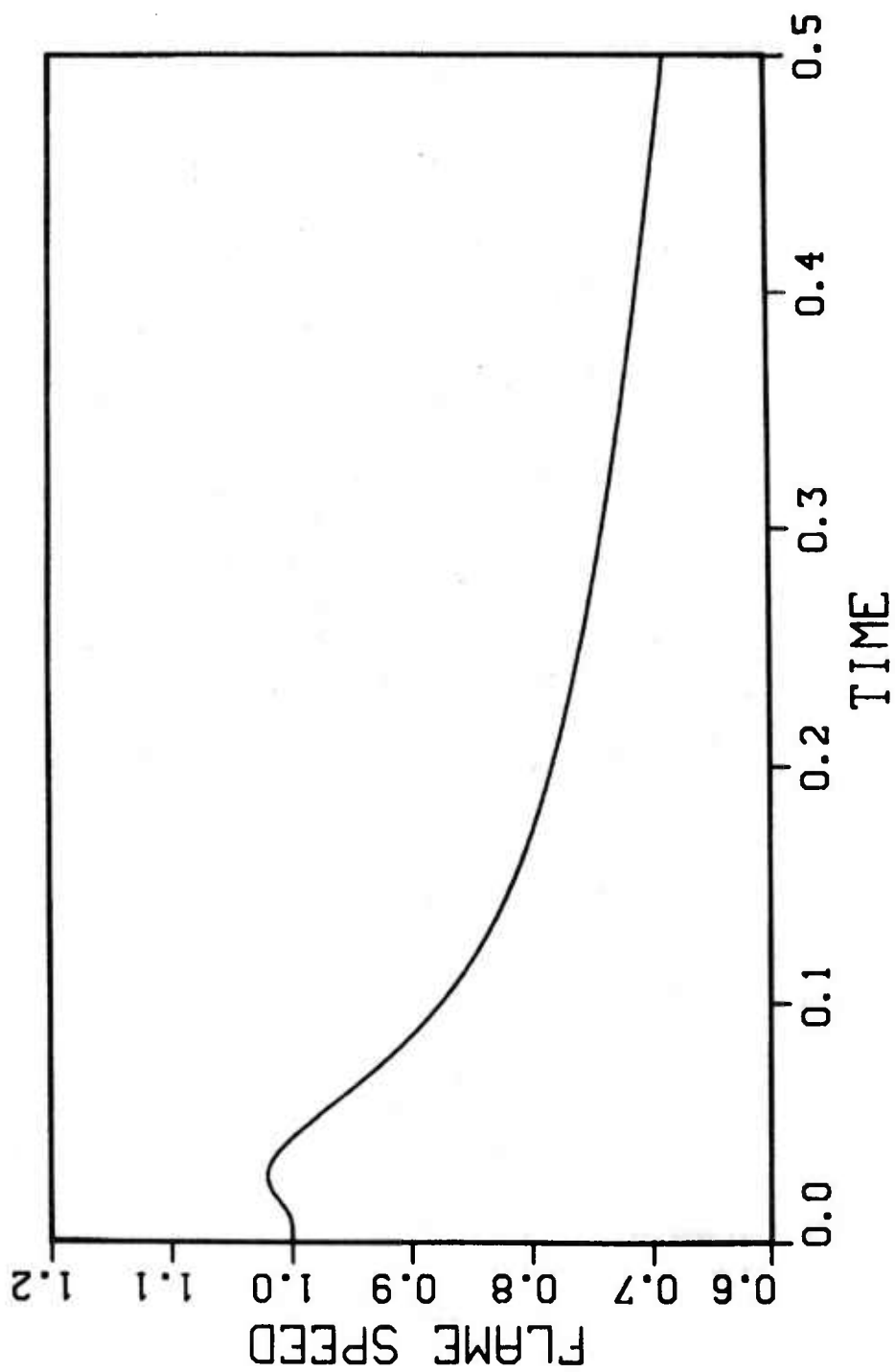


Figure 14. Case 5. Flame Speed Profile ($0 < \text{time} < 0.5$).

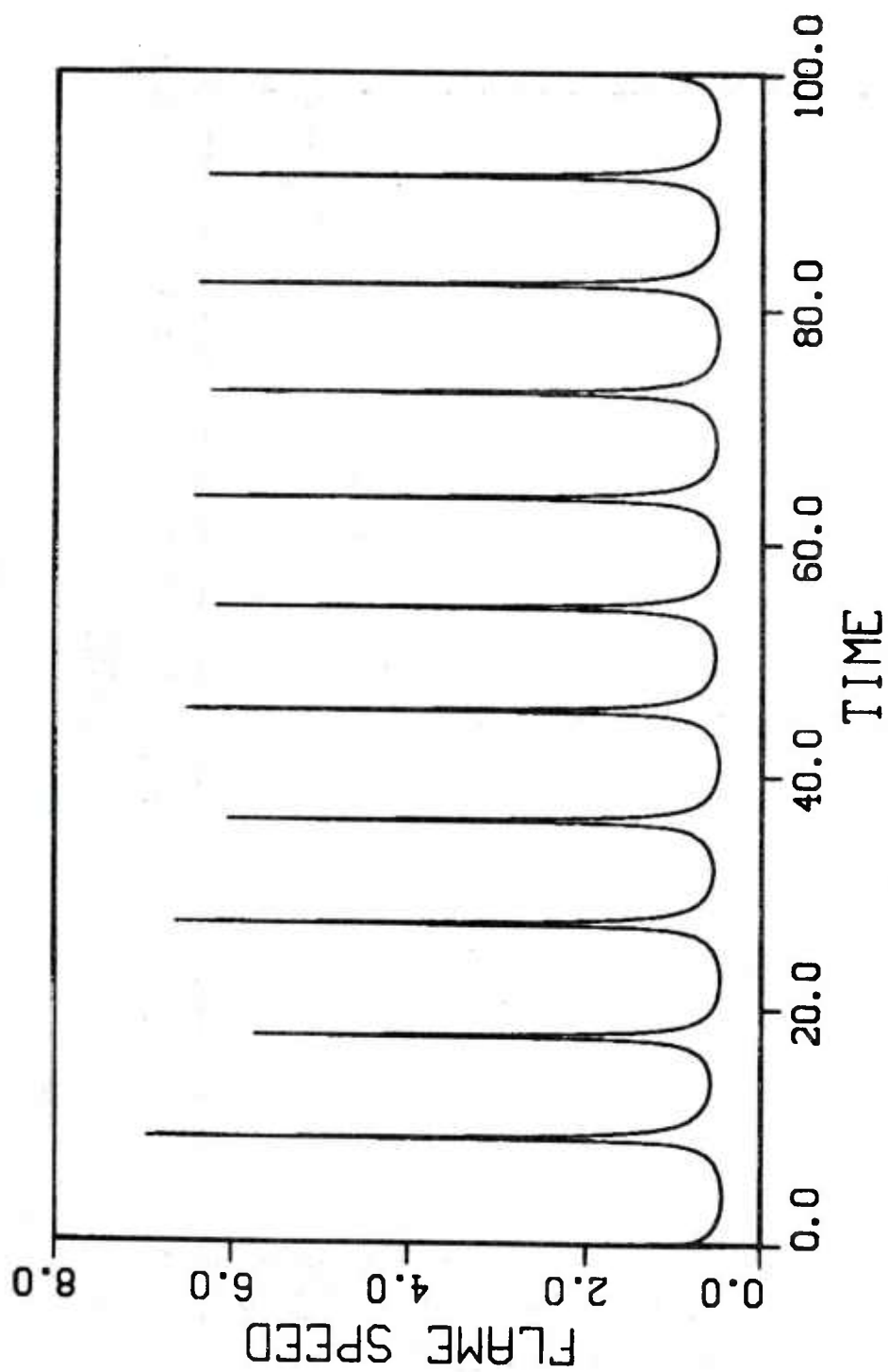


Figure 15. Case 5. Flame Speed Profile ($0 < \text{time} < 100$).

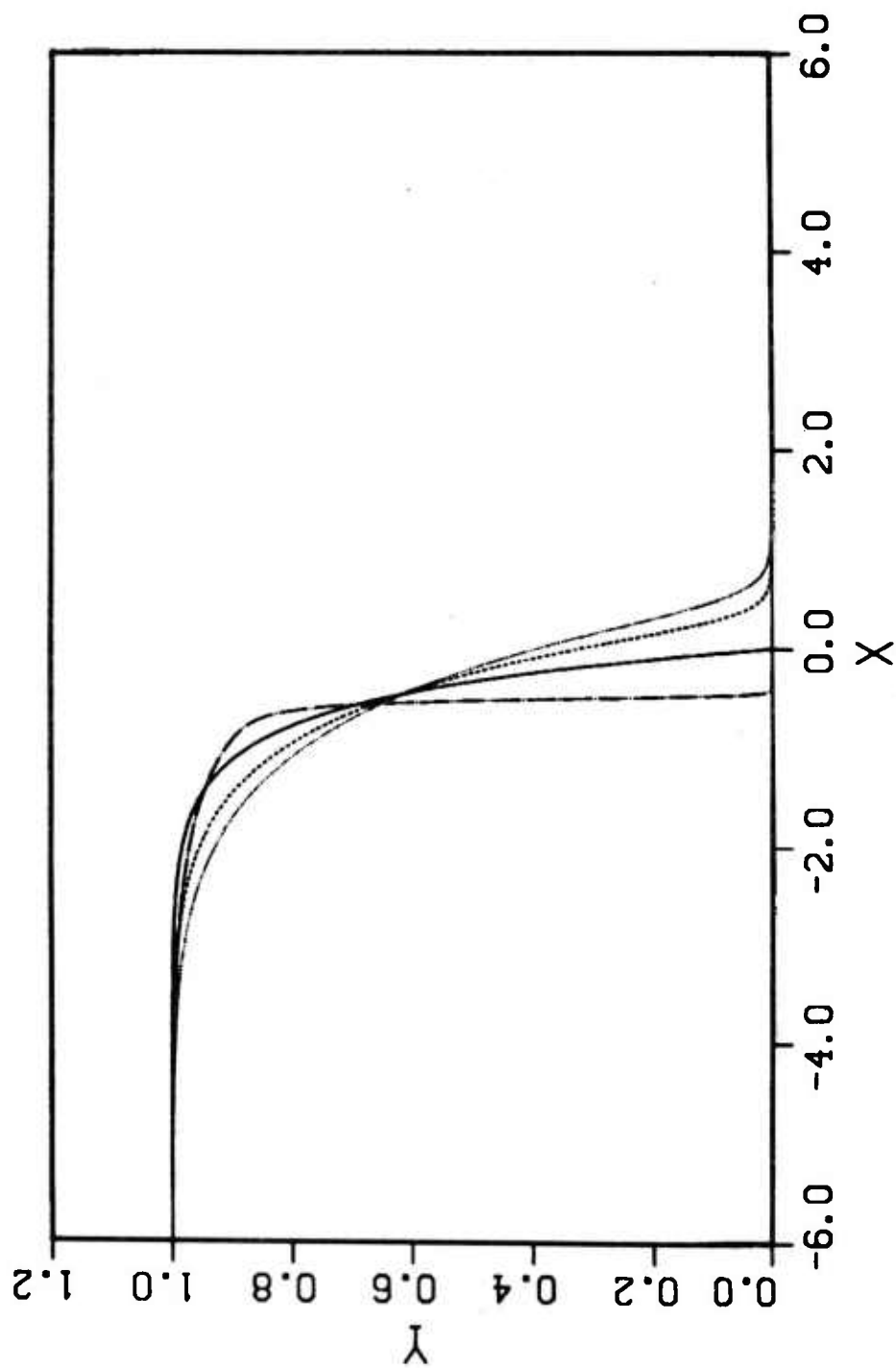


Figure 16. Case 5. Reactant Profile. Time = 0 (line). Time = 4.28 (dot). Time = 8.98 (chain-dot), Time = 13.483 (dash).

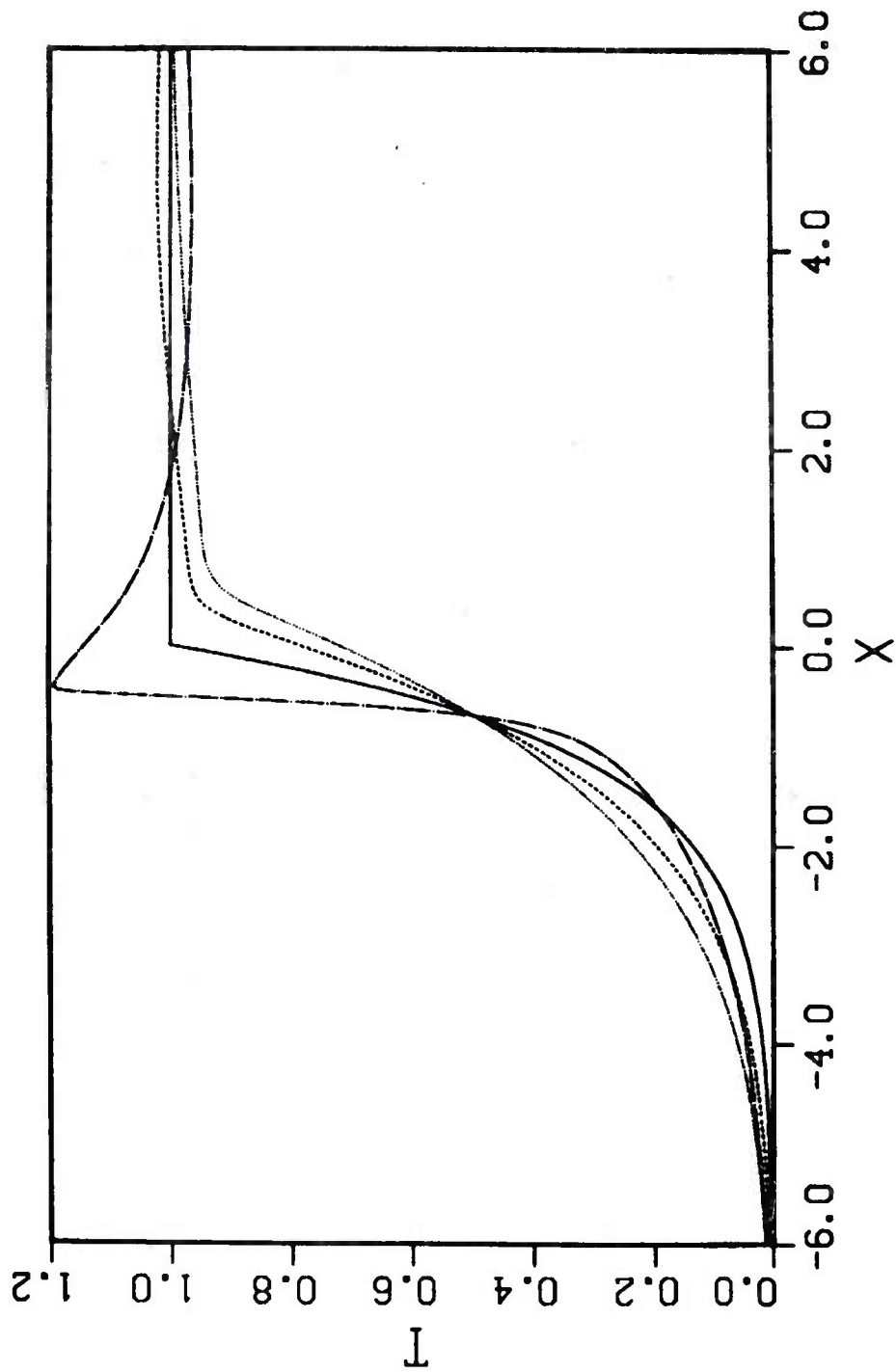


Figure 17. Case 5. Temperature Profile. Time = 0 (line). Time = 4.28 (dot). Time = 8.98 (chain-dot). Time = 13.483 (dash).

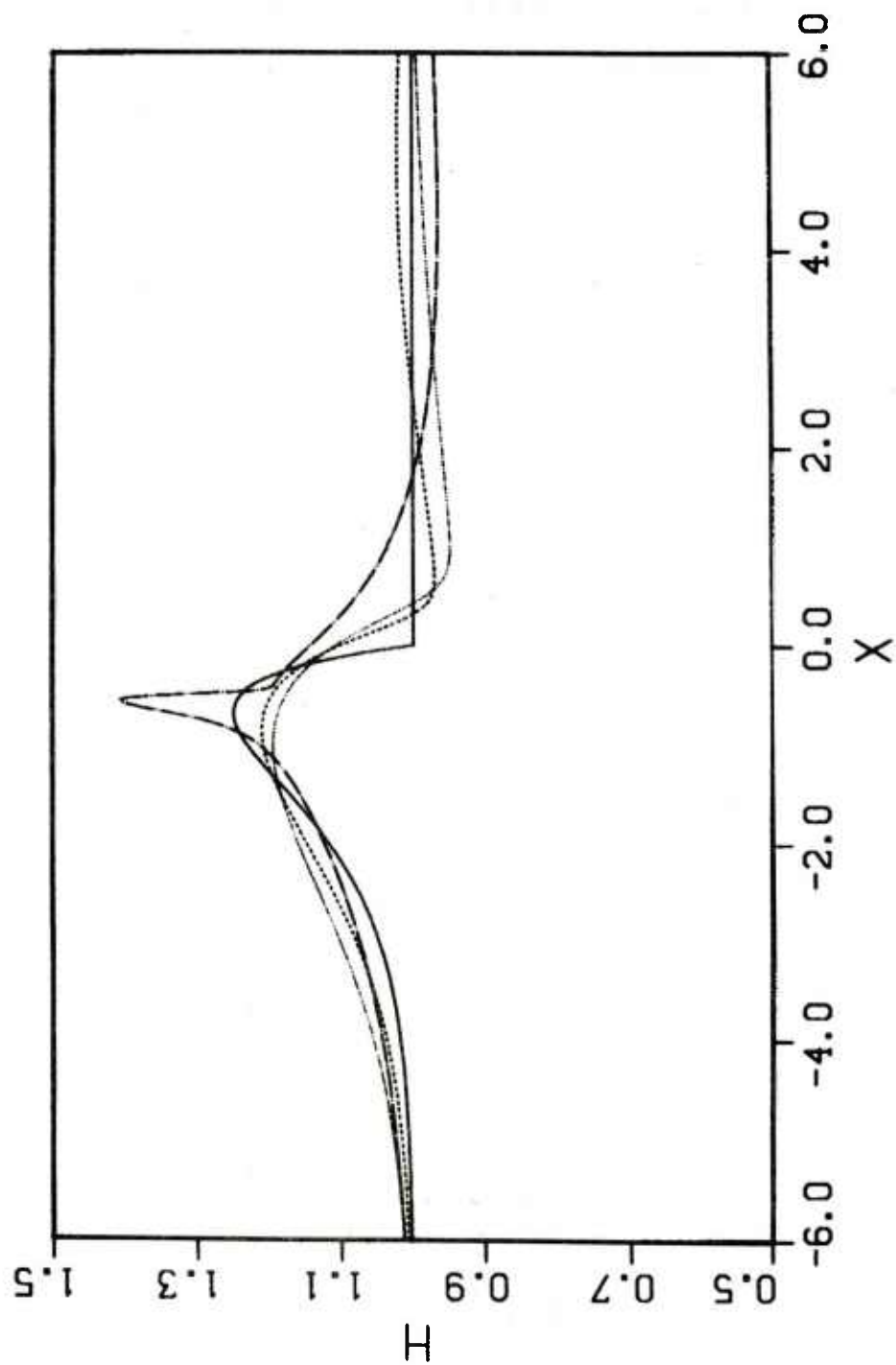


Figure 18. Case 5. Enthalpy Profile. Time = 0 (line). Time = 4.28 (dot). Time = 8.98 (chain-dot). Time = 13.483 (dash).

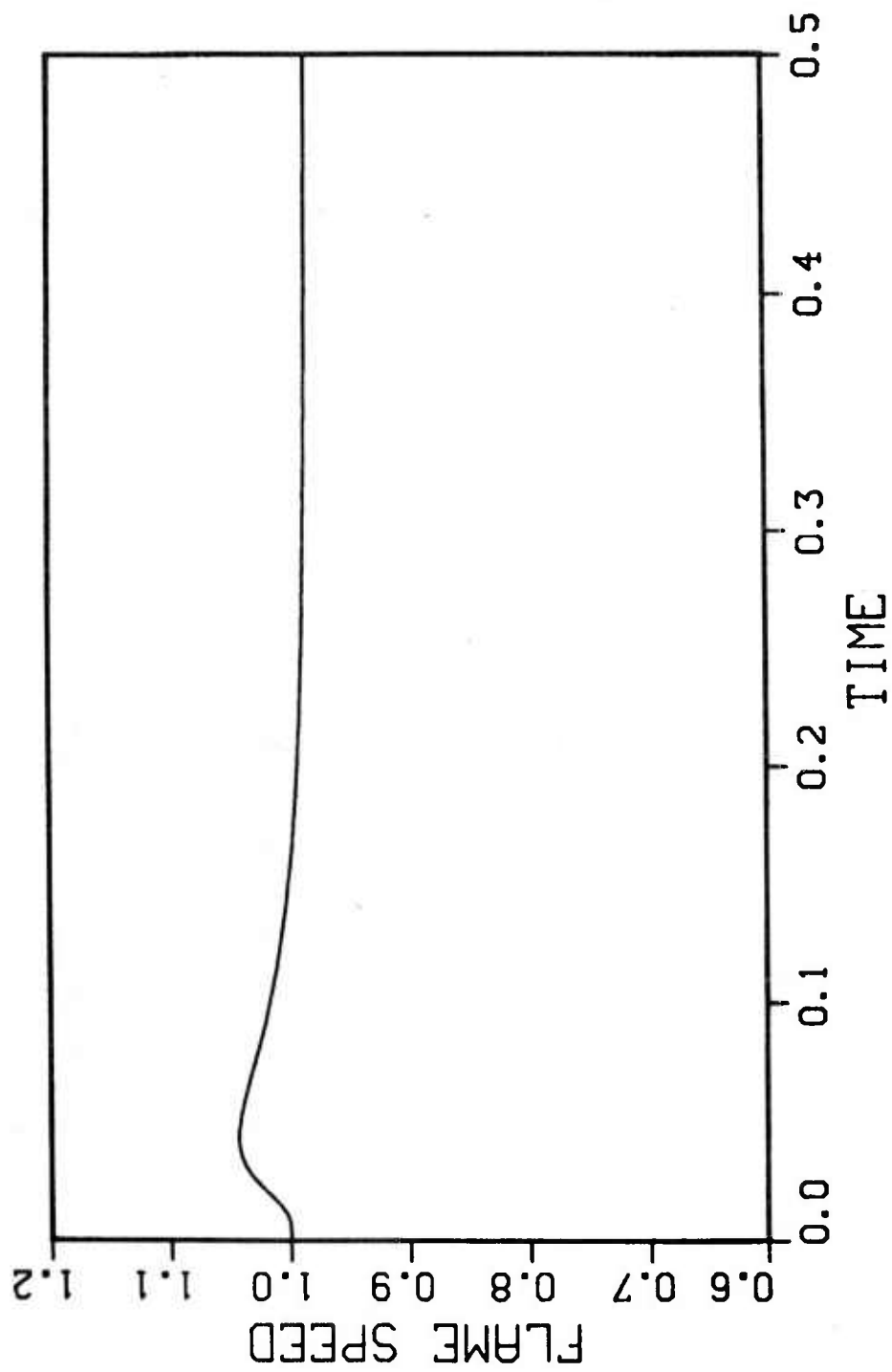


Figure 19. Case 6. Flame Speed Profile.

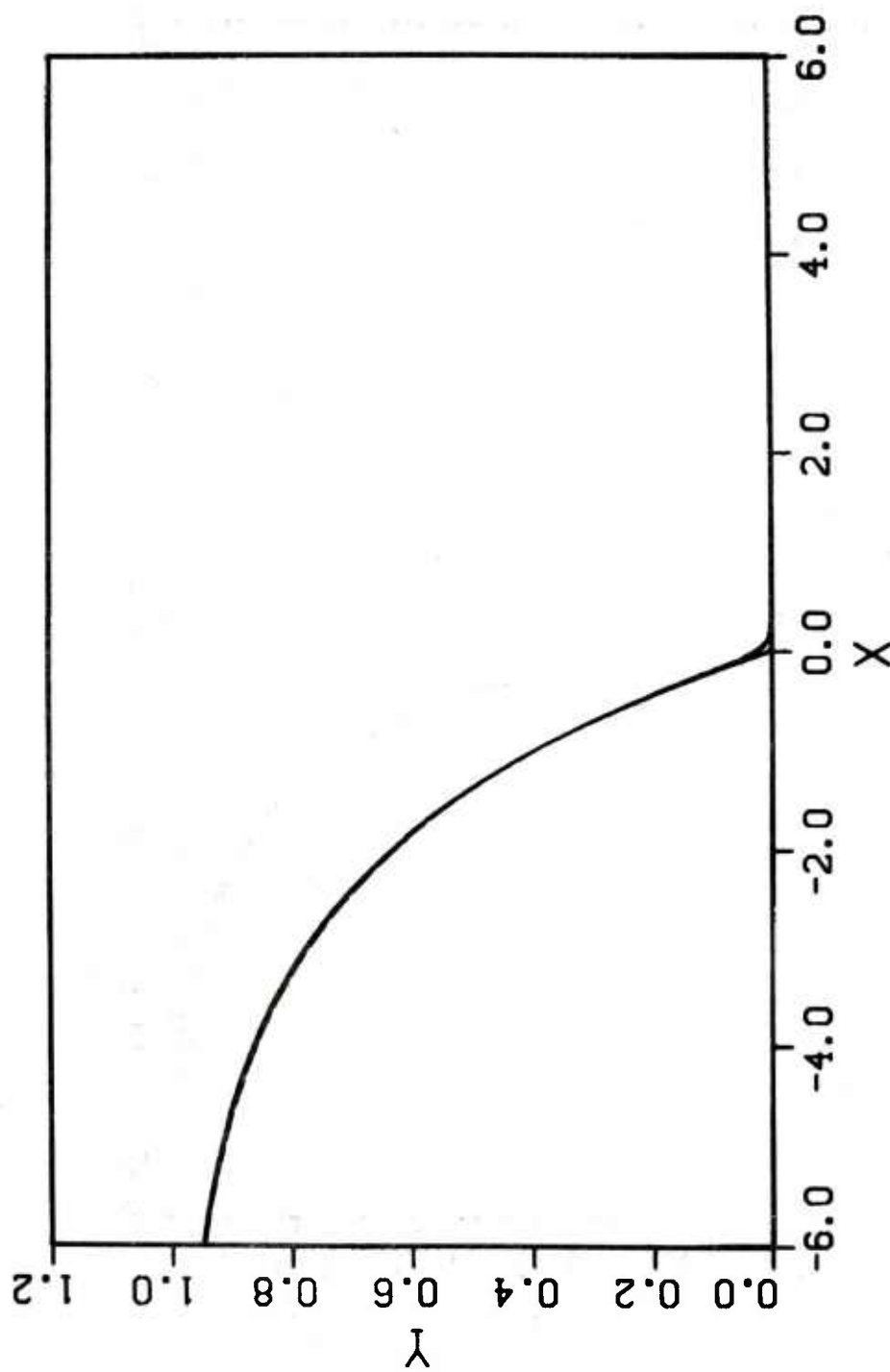


Figure 20. Case 6. Reactant Profile. Time = 0 (line). Time = 0.045 (dot). Time = 50 (chain-dot).

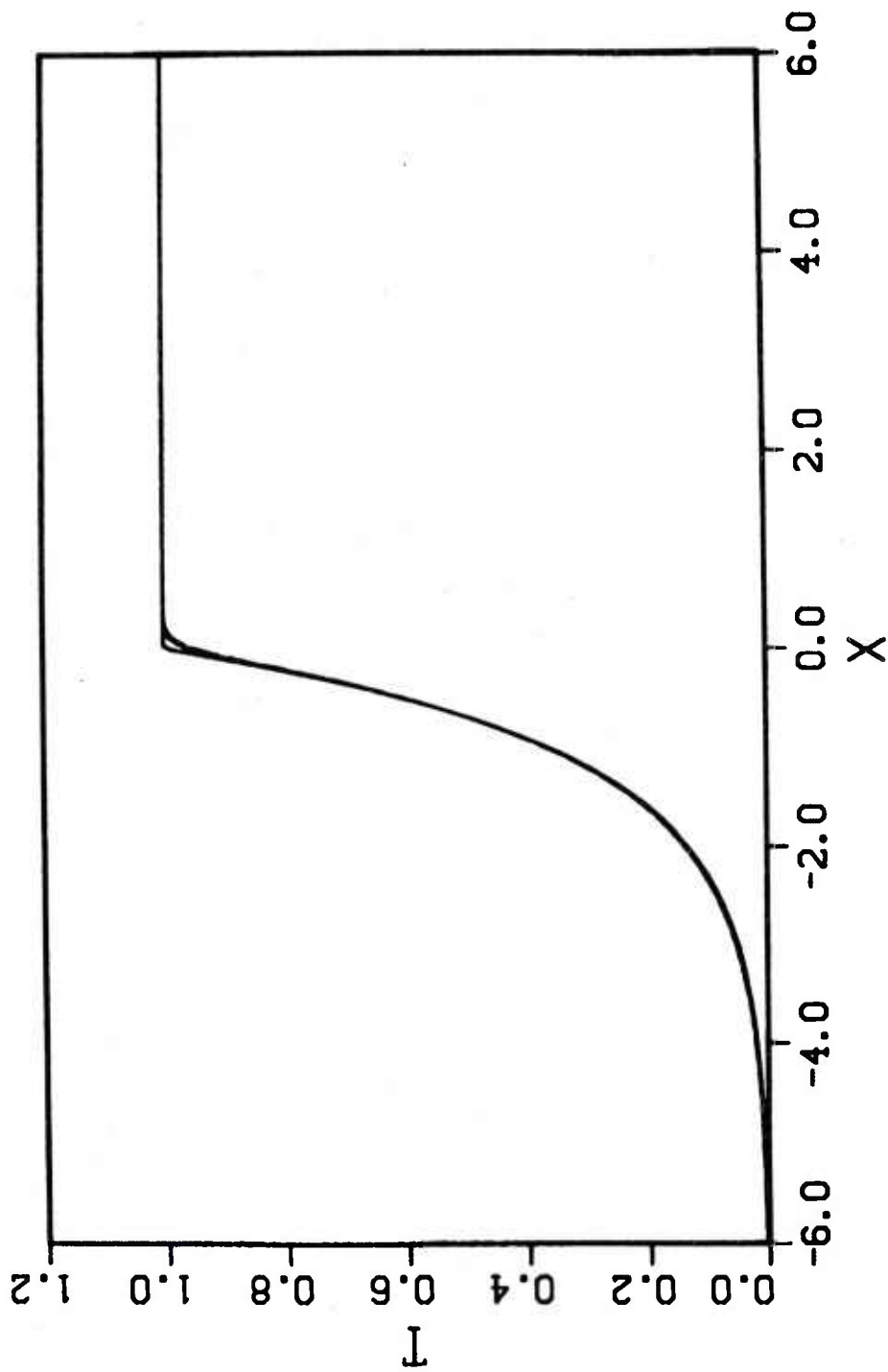


Figure 21. Case 6. Temperature Profile. Time = 0 (line). Time = 0.045 (dot). Time = 50 (chain-dot).

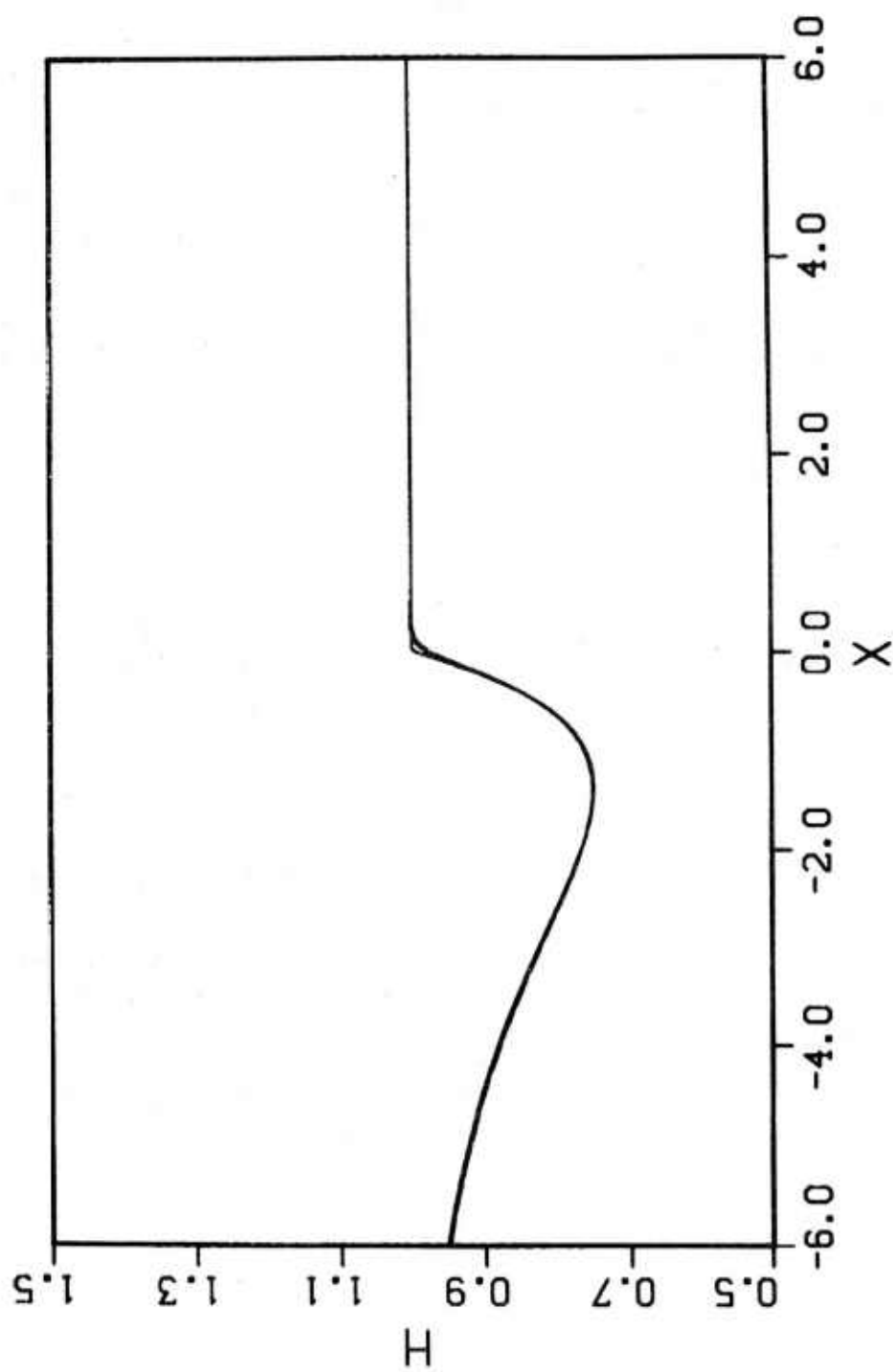


Figure 22. Case 6. Enthalpy Profile. Time = 0 (line). Time = 0.045 (dot). Time = 50 (chain-dot).

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