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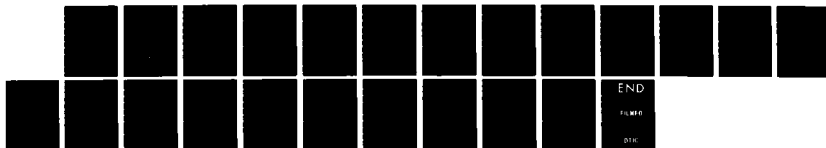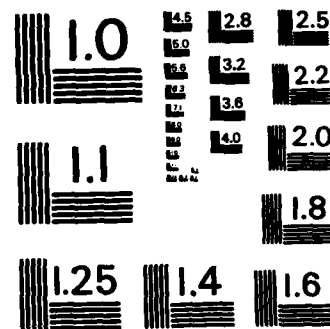   WASHINGTON DC   K KAILASANATH ET AL. 30 SEP 85
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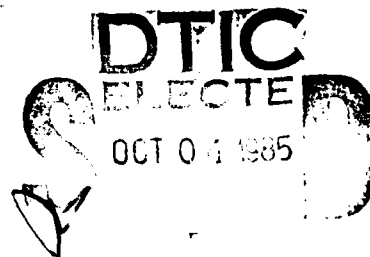NATIONAL BUREAU OF STANDARDS–1963–A

Effects of Curvature and Dilution on Unsteady, Premixed, Laminar Flame Propagation

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We have used a time-dependent, one-dimensional, Lagrangian model to study laminar flames in stoichiometric hydrogen-oxygen mixtures diluted with nitrogen. For stoichiometric hydrogen-air mixtures we have seen that a spherically expanding flame first decelerates until the velocity reaches a minimum value, and then it accelerates. For large radii, the burning velocity approaches the planar burning velocity. These same trends are also observed as the amount of diluent is increased. With increasing dilution, the flames reach their minimum velocities at larger times and larger radii. These observations are explained on the basis of flame stretch.

The spherical geometry results are compared to be results from another set of calculations in planar geometry. These show the minimum burning velocity reached by a spherical flame is less than that of a planar flame in the same mixture. In both planar and spherical geometries, the effect of increasing the dilution is to lower the burning velocities. Since the burning velocity is smaller in the spherical geometry, the flame can be extinguished (or quenched) with less dilution in the spherical geometry than in the planar geometry. We also discuss the implications of these results to laminar flame quenching and flammability limits.

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EFFECTS OF CURVATURE AND DILUTION ON UNSTEADY, PREMIXED, LAMINAR FLAME PROPAGATION

Introduction

In this paper, we present and discuss time-dependent calculations of one-dimensional laminar flames in stoichiometric hydrogen-oxygen mixtures diluted with nitrogen. We use these calculations to study the effects of curvature (or stretch) and dilution on flame propagation in pre-mixed gases. The results presented also have important applications to laminar flame quenching and flammability limits in the absence of external heat sinks.

Previous work on propane-air mixtures by Strehlow (1984) shows that rich mixtures exhibit a higher flame velocity at small radii than at large radii, while lean mixtures show a lower flame velocity at small radii than at large radii. In all cases, for large enough radii the flame velocity relaxes to the appropriate planar flame velocity. Strehlow attributes these effects to preferential diffusion of the lighter species and this has been verified by Frankel and Shivashinsky (1983) using an asymptotic a. lysis. More recently, Law (1984a; 1984b) used an asymptotic analysis to explain the behavior of stretched flames in rich and lean mixtures of methane and propane in air. These theoretical analyses are for either fuel-rich or fuel-lean conditions and use a simple phenomenology to represent the chemical kinetics.

This paper presents calculations of planar and spherically expanding flames in stoichiometric hydrogen-oxygen mixtures diluted with nitrogen.

The results presented here are obtained from numerical simulations, which use a time-dependent, one-dimensional, Lagrangian model (Kailasanath et al. 1982a). This numerical model was developed specifically to study the initiation, propagation and quenching of laminar flames. In addition to using a detailed chemical reaction mechanism, the model includes the effects of molecular diffusion, thermal conduction and thermal diffusion of the individual species considered. Because of the level of detail incorporated in the model, the spatial structure and temporal evolution of the flame structure can be highly resolved.

The Numerical Model

The numerical model solves the time-dependent conservation equations for mass, momentum and energy (Williams 1965; Oran and Boris 1981a). The model has been used for a variety of flame studies, including calculations of minimum ignition energies (Oran and Boris 1981b; Kailasanath et al. 1982b), quench volumes (Kailasanath et al. 1982b) and burning velocities (Kailasanath et al. 1982c). The model has a modular form and permits a wide variety of geometric, initial, boundary, and time varying energy input conditions. The algorithms representing the various chemical and physical processes are integrated separately and then asymptotically coupled by time-step splitting techniques (Oran and Boris 1981a). The convective transport is solved by the algorithm ADINC, a Lagrangian fluid dynamic algorithm which solves implicitly for the pressures (Boris 1979). The method gives an accurate representation of material interfaces and allows steep gradients in species and temperature to develop and be maintained. In addition to considering the thermal conduction and molecular diffusion processes in detail, the model also includes thermal diffusion. The chemical interactions are described by a set of nonlinear,

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coupled ordinary differential equations which are solved using a fully vectorized version of the selected asymptotic integration method CHEMEQ (Young and Boris 1977; Young 1980).

For this study we have used the hydrogen-oxygen reaction scheme (Burks and Oran 1981) which involves the eight reactive species H_2, O_2, H, O, OH, H_2O, HO_2, H_2O_2 and diluent, which is chosen to be nitrogen. The thermochemical properties of the various species involved are taken from the JANAF tables (Stull and Prophet 1971). The chemical reaction mechanism (given in Kailasanath et al. 1982a and 1982b) has been extensively tested and shown to give good results. Burks and Oran (1981) showed that the results computed with this mechanism compare well with experimentally observed induction times, second explosion limits and the temporal behavior of reactive species. Oran et al. (1982) have shown that the mechanism coupled to a convective transport algorithm gives good results in the simulation of the conditions behind a reflected shock. The laminar burning velocities calculated using the mechanism are in agreement with experimental data (Kailasanath et al. 1982c).

For the calculations presented below, the model was configured with an open boundary at one end to simulate an unconfined system. Most of the calculations were done in a spherically symmetric one-dimensional geometry. Other calculations were done assuming a planar configuration. All the calculations are for stoichiometric mixtures of hydrogen and oxygen at an initial temperature and pressure of 298 K and 1 atmosphere, respectively. The amount of nitrogen was varied, thereby varying the dilution.

Results and Discussion

Estimation of Burning Velocity

For either thin or planar flames, the instantaneous normal burning

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velocity can be calculated from the flame velocity if we know the velocity of the unburnt gases ahead of the flame. For planar flames, the velocity of the unburnt gases ahead of the flame is constant, as shown in Fig. 1, where the spatial variation of the flow velocity and the temperature across the flame is shown for a hydrogen-air mixture. Hence the burning velocity can be unambiguously determined as the difference between the flame velocity and the flow velocity ahead of the flame,

$$V_b = V_f - V_{flow} \quad .$$

For a thin flame, a similar definition is adequate. However, when the flame has a finite thickness and is curved (as for a spherically expanding flame), the appropriate definitions for the location of the flame front and the fluid velocity of the unburnt gases are ambiguous. This can be seen in Fig. 2, in which the spatial variation of the flow velocity and the temperature across a spherical flame in a hydrogen-air mixture is shown. The fluid velocity reaches a maximum within the flame and then decreases ahead of the flame.

For the flames studied in this paper, two reference fluid velocities have been chosen for estimating the burning velocity. One of them is the maximum fluid velocity (V_{max}) in the system and the other is the fluid velocity of the unburnt gases (V_{300}) corresponding to the first location ahead of the flame with temperature of 300 K. The lower estimate for the burning velocity is obtained as ($V_f - V_{max}$) and the upper estimate as ($V_f - V_{300}$). For a planar flame in which the fluid velocity ahead of the flame is constant and the same as the maximum fluid velocity, the two estimates for the burning velocity are identical.

Effects of Curvature

In the first set of calculations, a spherically expanding flame in

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a stoichiometric hydrogen-air (actually $H_2:O_2:N_2$ / 2:1:4) mixture was studied. In these simulations, energy was deposited linearly over a fixed period of time at the center of a spherically symmetric system. The radius of energy deposition was larger than the quench-radius (Kailasanath et al. 1982b) and was held constant. We then tracked the spatial location of the flame kernal as a function of time, and used this to calculate the apparent flame velocity as a function of time. The results of such a calculation are shown in Fig. 3. The flame velocity (V_f) initially decreases with time until it reaches a minimum value, and then it increases. The figure also shows the maximum fluid velocity (V_{max}) of the system and the fluid velocity of the unburn gases (V_{300}) corresponding to the first location ahead of the flame with temperature of 300 K. With increasing radii, the difference between the two fluid velocities decreases. For very large radii (not shown in the figure), there is an unambiguous burning velocity since the two fluid velocities approach the same value. This estimated burning velocity approaches both the experimental value and the value determined from a separate planar one-dimensional calculation.

Effects of Dilution

We also performed a series of calculations in which the amount of diluent was varied. The results of one such calculation, for the $H_2:O_2:N_2$ / 2:1:7 mixture, is shown in Fig. 4. Increasing the amount of diluent does not change the observed trends: the flame velocity and the burning velocity decrease with increasing radii, attain a minimum value and then increase with increasing radii. This calculation and the results shown in Fig. 5 for the $H_2:O_2:N_2$ / 2:1:10 case show that it takes longer for the flame to reach the minimum flame velocity as dilution increases. For the 2:1:10 mixture, we expect the flame velocity to increase again at larger

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radius following the trend seen in the other two mixtures. For this mixture the burning velocity corresponding to the minimum flame velocity is .30 - .35 m/s, where as the calculated burning velocity for a planar flame in the same mixture is .85 - .90 m/s. Thus the burning velocity of a spherical flame corresponding to the minimum value of the flame velocity is smaller than that of a planar flame in the same mixture. We have observed this trend in all of the stoichiometric mixtures we have studied.

Some of the more dilute mixtures studied do not support spherical flame propagation. One such case is the $H_2:O_2:N_2/$ 2:1:13 mixture, in which the flame velocity does not level off but continues to decrease until the flame dies. Figure 6 shows V_f, V_{max} and V_{300} as a function of time for this case. We varied the radius of energy deposition, the amount of energy input and the mode of energy input. In all cases the flame died after propagating for a short time.

When we modelled flame propagation in the planar geometry, we observed significiant burning velocities for a wider range of mixtures than in the spherical geometry. For example, the burning velocity was between .34 and .40 m/s for the $H_2:O_2:N_2$ / 2:1:13 mixture. As mentioned above, this mixture did not support spherical flame propagation.

Effects of Stretch

The observed time histories of the flame velocity can be explained on the basis of stretch (due to flow divergence) and chemical kinetics. First, consider the initial deceleration of V_f in spherical geometry. Initially, due to flow divergence the energy released in chemical reactions does not balance the energy conducted and diffused into the unreacted mixture. Because of this, the flame velocity and temperature

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decrease as the flame expands. The decrease in the flame temperature decreases the energy release rate, which leads to a lower flame velocity, and so on. However, this process does not continue indefinitely because the stretch effect decreases with increasing radii. Because of this effect a minimum flame velocity is observed in spherical flame propagation. As the radius of the flame increases further, the energy released in chemical reactions is larger than the energy conducted and diffused into the unburnt mixture. Now the flame velocity increases with increasing radii until a balance is attained between the energy released by chemical reactions and the energy conducted and diffused into the unburnt mixture ahead of the flame. Such a balance occurs for large radii and then the flame propagates as if it were planar.

The above observations are verified by the temperatures calculated in the numerical simulations. The time history of the maximum temperature in a spherically expanding flame in a hydrogen-air mixture is shown in Fig. 7. The maximum temperature corresponding to the minimum velocity spherical flame is significantly lower than that of a planar flame in the same mixture. After reaching a minimum, the flame temperature increases and tends towards the temperature corresponding to a planar flame 'n the same mixture.

The actual radius at which the minimum flame velocity occurs and the radius at which the effect of stretch becomes negligible depend on the flame thicknesss. Since the flame thickness increases with increasing dilution, a flame in a more dilute mixture will have to propagate to a larger radius in order to overcome the effects of stretch. This explains the observation made above which showed that the minimum flame velocity is reached at a later time (and a larger radius) as dilution is increased.

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Not only is the minimum flame velocity reached later, but the magnitude of the velocity and the flame temperature are smaller. Therefore by increasing the dilution, one can obtain a mixture which will be quenched by endothermic reactions before it can overcome the effects of stretch. This appears to be the case with the $H_2:O_2:N_2$ / 2:1:13 mixture.

Summary and Conclusions

We have studied flames in stoichiometric hydrogen-oxygen mixtures diluted by nitrogen in spherical and planar geometries using time-dependent, one-dimensional numerical simulations. The model includes a full description of the eight reactive species involved in hydrogen-oxygen kinetics plus detailed models for the chemical kinetics, thermal conduction, and thermal and molecular diffusion processes. These studies have led to a number of interesting observations and important questions on flame behavior.

We have seen that, in a stoichiometric hydrogen-air mixture, the flame velocity of spherically expanding flames first decreases with increasing radii, and then increases. For large radii, the burning velocity approaches the planar burning velocity. These same trends are observed when the amount of diluent is increased. However, with increase in dilution, the minimum flame velocity is reached at a later time and at a larger radius. Comparing these spherical geometry results to another set of calculations in planar geometry shows that the minimum burning velocity of a spherical flame is less than that of a planar flame in the same mixture.

In both planar and spherical geometries, the effect of increasing the dilution is to lower the burning velocities. Since the burning

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velocity is smaller in the spherical geometry, the flame can be exting-
uished (or quenched) with less dilution in the spherical geometry than in
the planar geometry. The existence of a quench-radius and a minimum
ignition energy in the absence of heat or radical loss to walls or other
external sinks has already been demonstrated (Kailasanath et al. 1982b).
The results presented here indicate that such "self-quenching" also
depends on the geometry or curvature.

The time histories of the flame velocity are controlled by stretch
(due to flow divergence) and energy release by chemical reactions. The
maximum temperature of a spherically expanding flame exhibits the same
trends as the flame velocity. The actual radius at which the minimum
flame velocity occurs and the radius at which the effect of stretch
becomes less important depends on the thickness of the flame. The thick-
ness of the flame increases with increasing dilution. Therefore a more
dilute flame will have to propagate to a larger radius in order to over-
come the effects of stretch. The minimum flame velocity and the flame
temperature decrease with increasing dilution. Therefore by increasing
the dilution one can obtain a mixture which will be quenched by endo-
thermic reactions before it can overcome the effects of stretch. This
appears to be the case with the $H_2:O_2:N_2/2:1:13$ mixture which does
not support spherical flame propagation.

It has been shown experimentally that the addition of inert gases
to confined fuel-air mixtures can cause the flammability limits to become
narrower (Zabetakis 1965; Strehlow 1984). That is, by adding sufficient
amounts of an inert gas we can obtain a mixture which does not support
flame propagation. Our calculations support this conclusion even though
we do not include any heat or radical loss to the confining walls. The

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actual limits obtained might, however, depend on parameters such as the method of initiation, the duration of energy deposition and the geometry of the system. By systematically varying these parameters as well as the stoichiometry, the numerical simulations can be used to help answer questions regarding the existence of fundamental flammability limits.
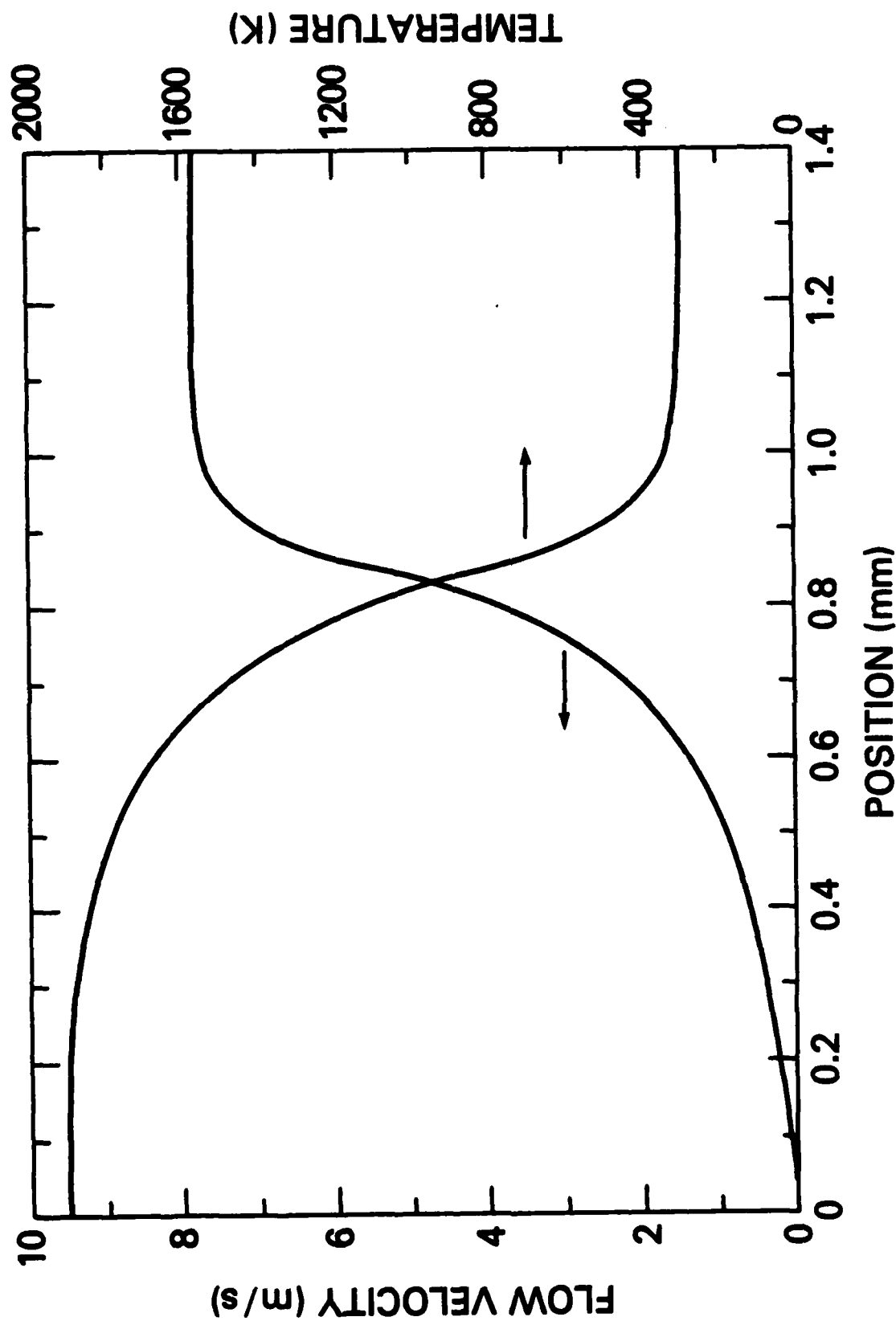
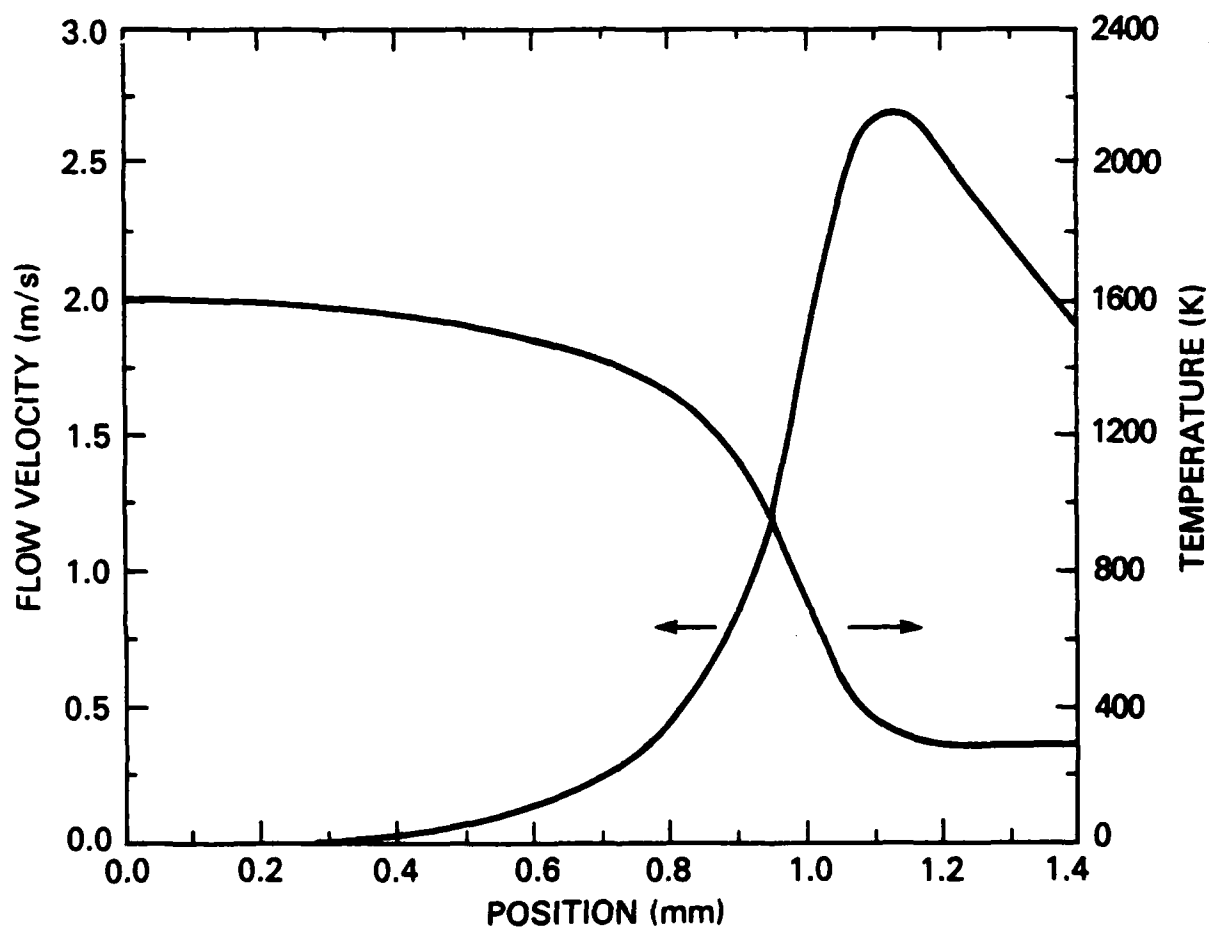Fig. 1 The flow velocity and temperature profiles in a planar flame propagating in a $H_2:O_2:N_2/2:1:4$ mixture.

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Fig. 2 The flow velocity and temperature profiles at a particular time in a spherically expanding flame in a $H_2:O_2:N_2/2:1:4$ mixture.
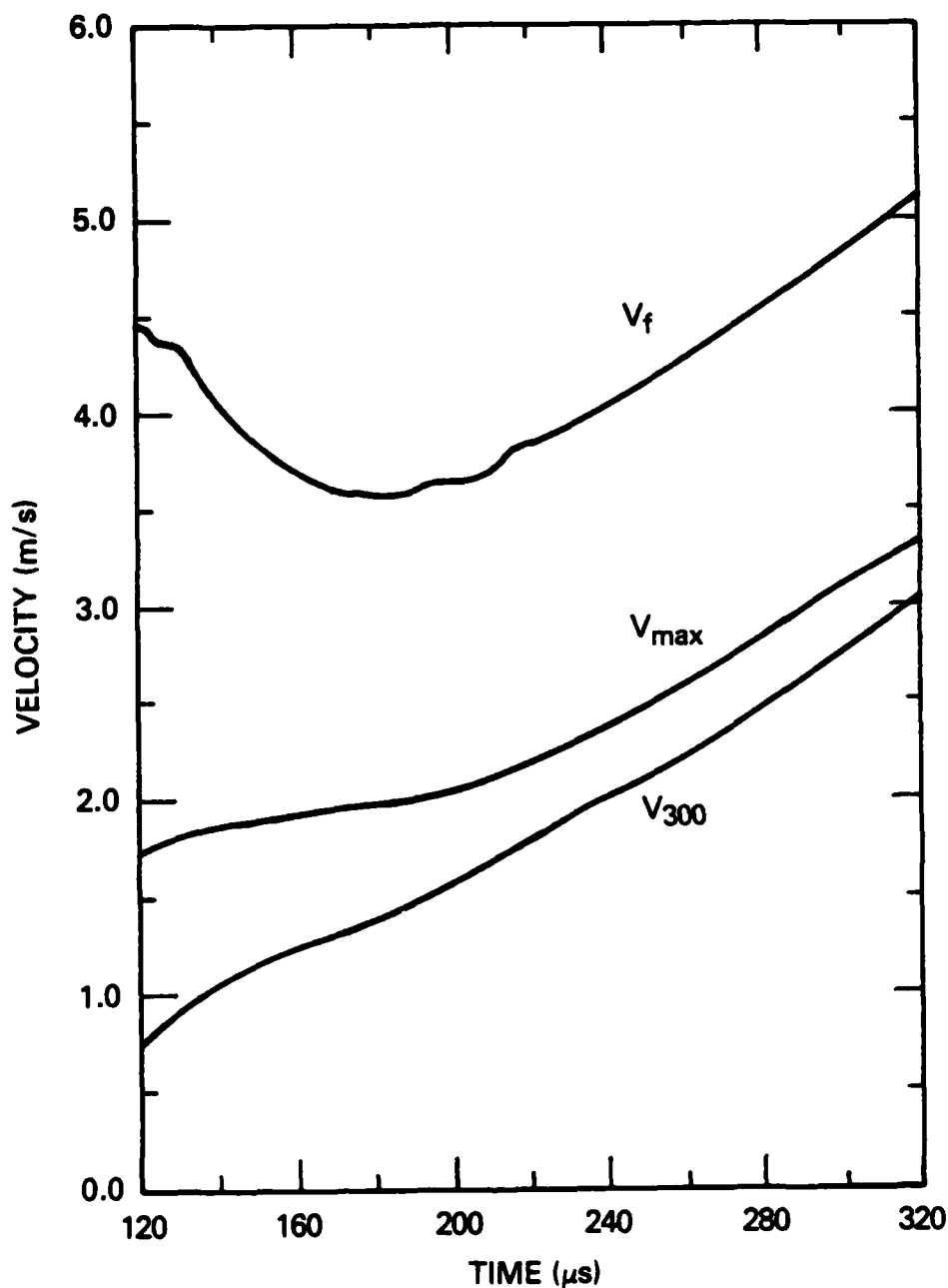
Fig. 3 Time history of the propagation of a spherically expanding flame in a $H_2:O_2:N_2/2:1:4$ mixture. The flame velocity is denoted V_f, the maximum fluid velocity is V_{max}, and the velocity of the first position ahead of the flame with a temperature of 300 K is V_{300}.
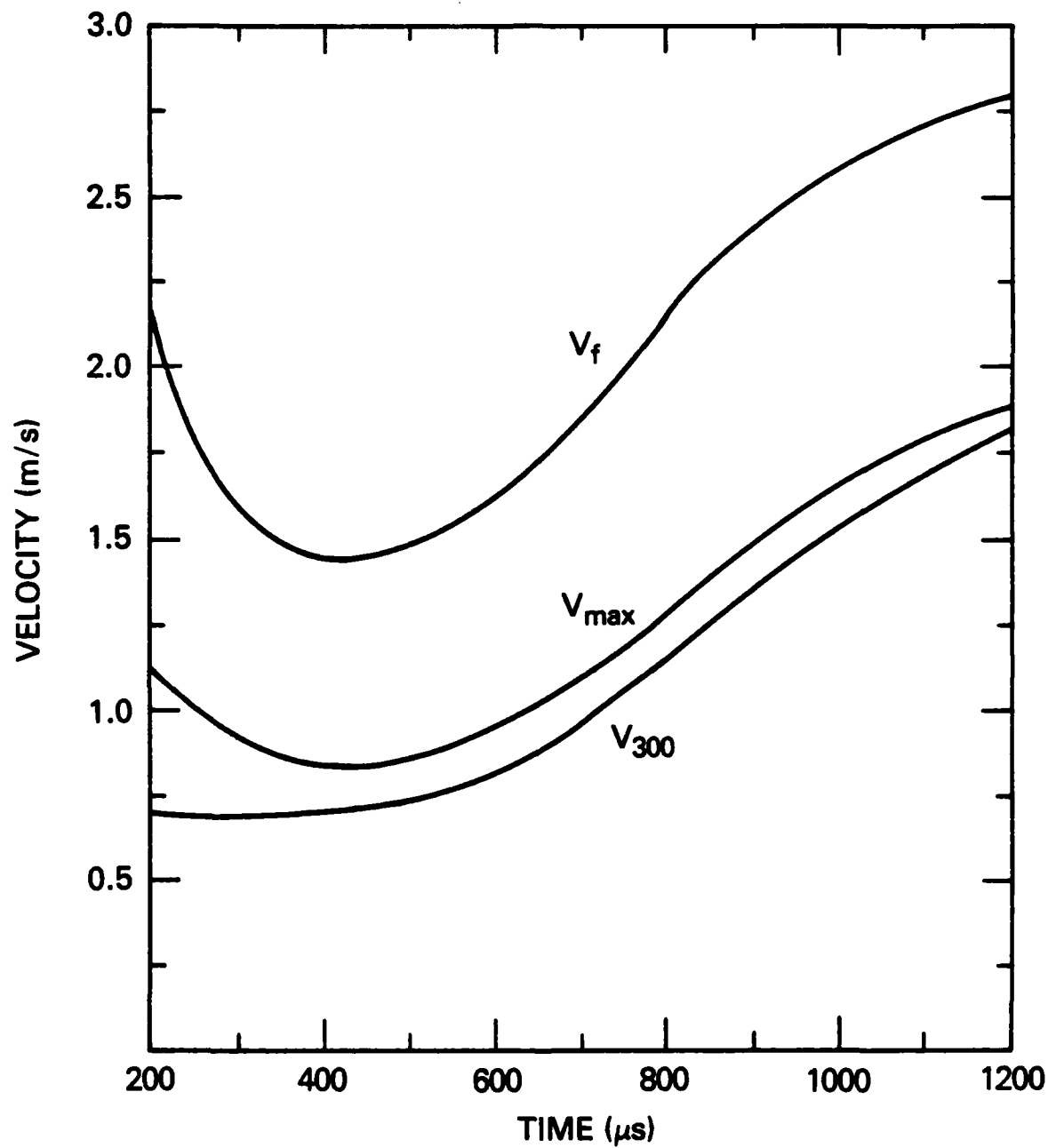
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Fig. 4 Time history of the propagation of a spherically expanding flame in $H_2:O_2:N_2/2:1:7$ mixture. See Fig. 3 for legends.
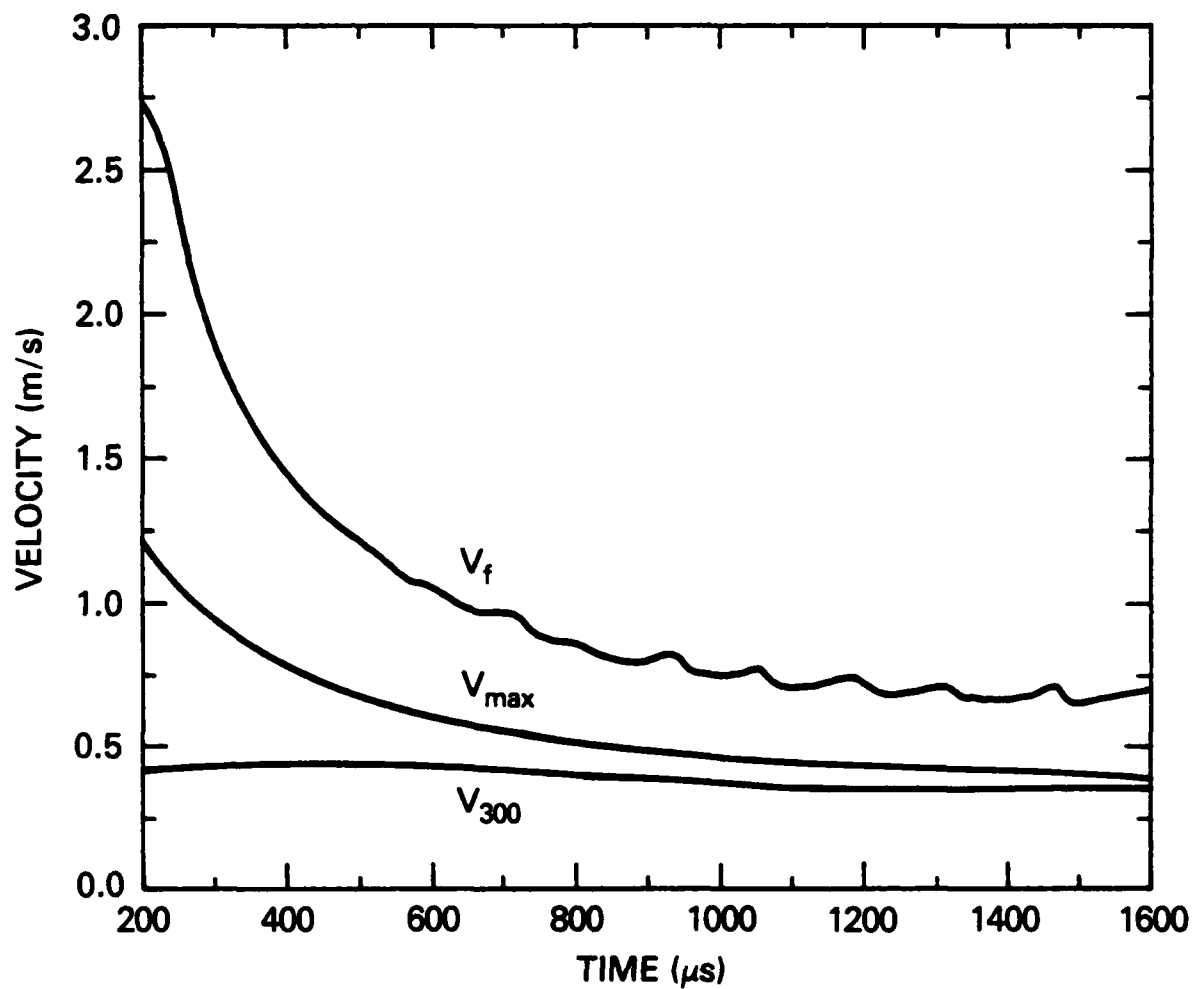
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Fig. 5 Time history of the propagation of a spherically expanding flame

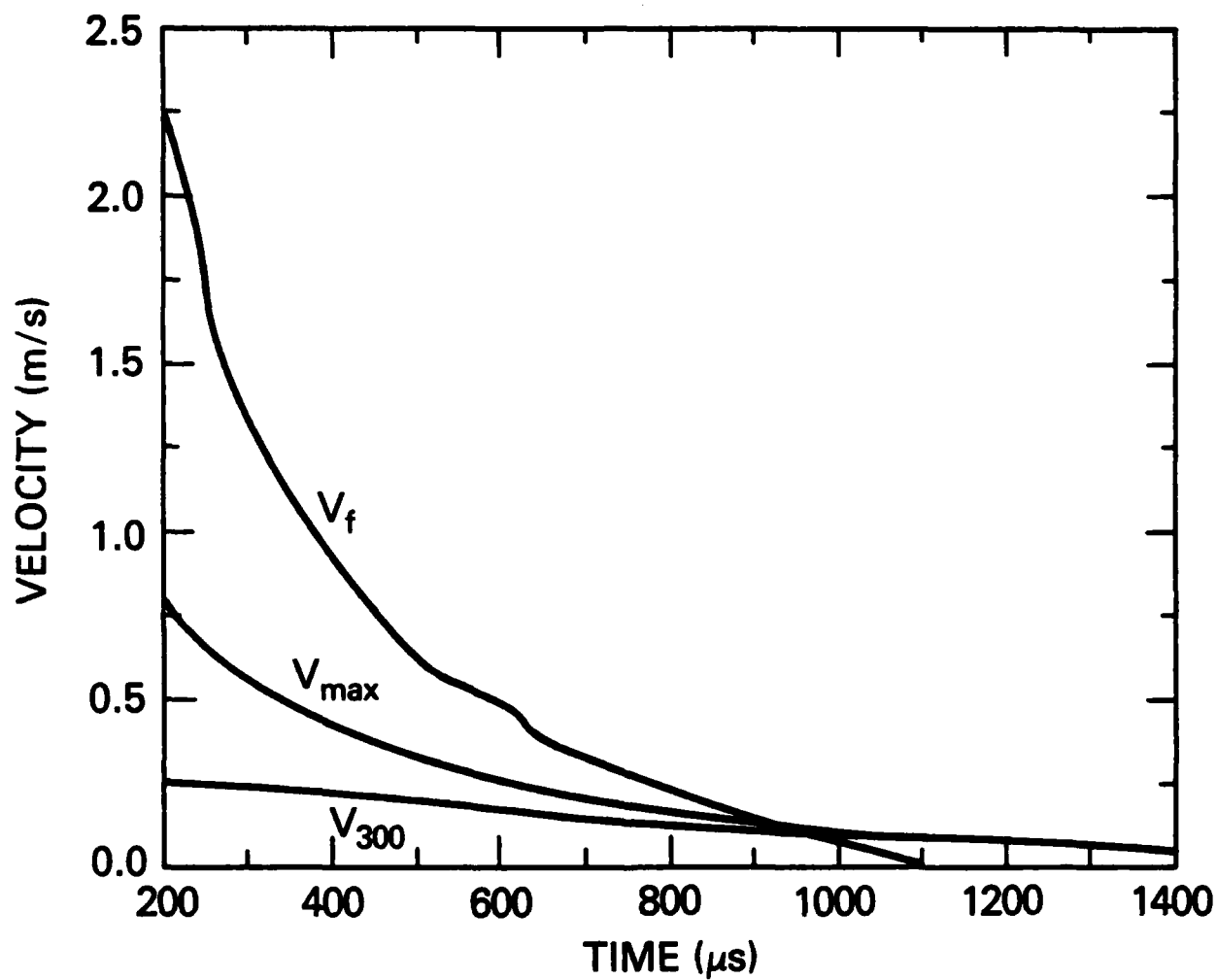in $H_2:O_2:N_2/2:1:10$ mixture. See Fig. 3 for legends.

Fig. 6 Time history of the propagation of a spherically expanding flame in a $H_2:O_2:N_2/2:1:13$ mixture. See Fig. 3 for legends.
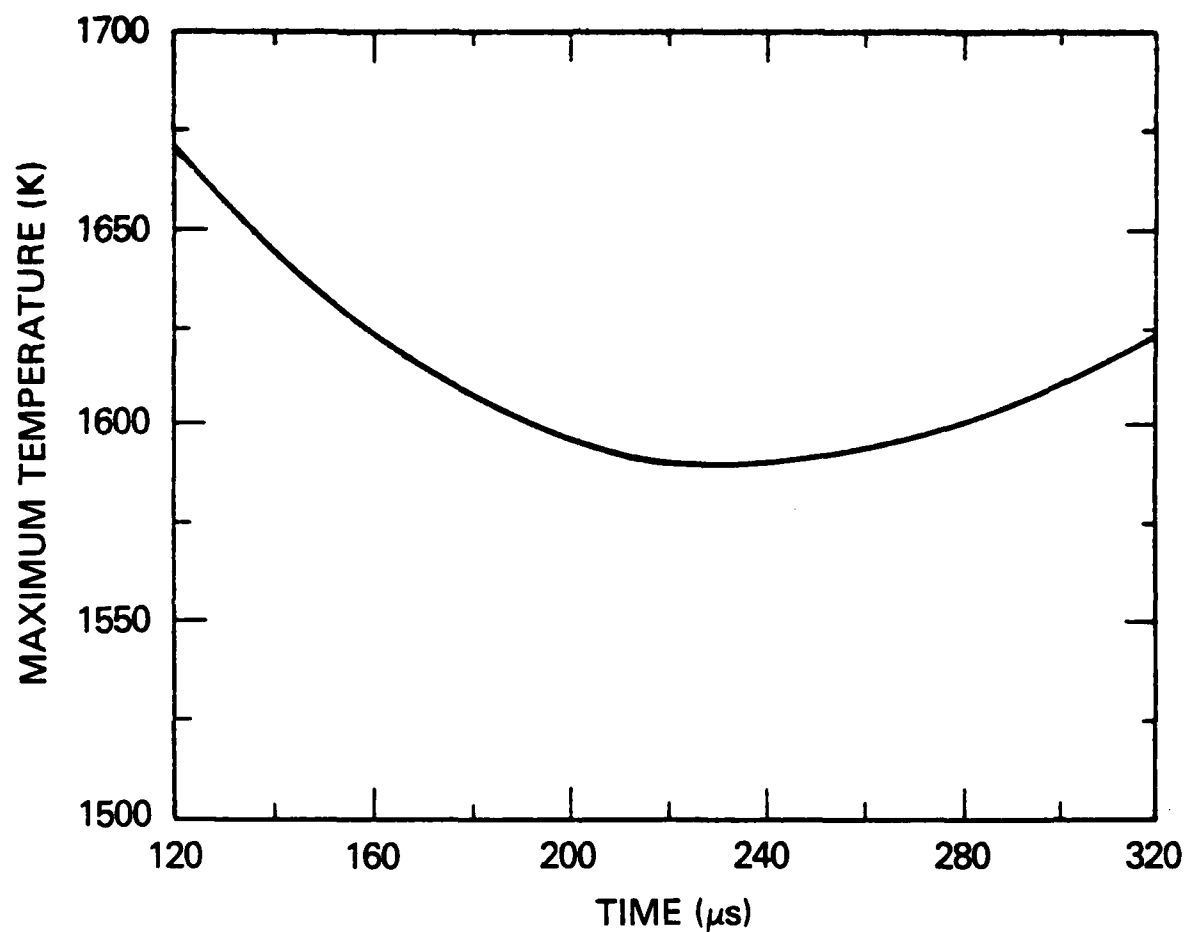
Fig. 7 Time history of the maximum temperature of a spherically expanding flame in a $H_2:O_2:N_2/2:1:4$ mixture.

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References

Boris, J.P. (1979) ADINC: An implicit lagrangian hydrodynamics code, NRL
Memorandum Report 4022, Naval Research Laboratory, Washington, D.C.
AD A070 361

Burks, T.L. and Oran, E.S. (1981) A computational study of the chemical
kinetics of hydrogen combustion, NRL Memorandum Report 4446, Naval
Research Laboratory, Washington, D.C. (AD-A094 348)

Frankel, M.L. and Shivashinsky, G.I.(1983) On effects due to thermal
expansion and Lewis number in spherical flame propagation, Comb. Sci.
Tech. 31, 131-138.

Kailasanath, K., Oran, E.S. and Boris, J.P. (1982a) A one-dimensional
time-dependent model for flame initiation, propagation and quenching,
NRL Memorandum Report No. 4910, Naval Research Laboratory, Washington,
D.C. (AD-A119748)

Kailasanath, K., Oran, E.S. and Boris, J.P. (1982b) A theoretical study of
the ignition of premixed gases, Combust. Flame. 47, 173-190.

Kailasanath, K., Oran, E.S. and Boris, J.P. (1982c) Time-dependent simu-
lation of flames in hydrogen-oxygen-nitrogen mixtures, in Numerical
Methods in Laminar Flame Propagation, p. 152, Friedr. Vieweg & Sohn,
Wiesbaden.

Law, C.K. (1984a) Heat and mass transfer in combustion: fundamental con-
cepts and analytical techniques, Prog. Energy Combust. Sci. 10,
295-318.

Law, C.K. (1984b) Dynamics of stretched flames, Abstracts of the Eastern
Section of the Combustion Institute, Fall 1984 Technical Meeting,
pp. C1-C11, The Combustion Institute, Pittsburgh, Pa.

Oran, E.S. and Boris, J.P. (1981a) Detailed modelling of combustion processes. _Prog. Energy Comb. Sci._ 7, 1-71.

Oran, E.S. and Boris, J.P. (1981b) Theoretical and computational approach to modelling flame ignition, _Prog. Astro. Aero._ 76, 154-171.

Oran, E.S., Young, T.R., Boris, J.P. and Cohen, A. (1982) Weak and strong ignition. I. Numerical simulations of shock tube experiments., _Combust. Flame_ 48, 135-148.

Strehlow, R.A.(1984) _Combustion Fundamentals_, Mcgraw-Hill, New York.

Stull, D.R. and Prophet, H. (1971) JANAF Thermochemical Tables, NSRDS-NBS 37, 2nd Ed., National Bureau of Standards, Gaithersburg, Md. AD-D095 223

Williams, F.A. (1965) _Combustion Theory_, Addison-Wesley, Reading, Ma., p.2.

Young, T.R. and Boris, J.P. (1977) A numerical technique for solving stiff ordinary differential equations associated with chemical kinetics of reactive-flows problems. _J. Phys. Chem._ 81, 2424-2427.

Young, T.R. (1980) CHEMEQ - a subroutine for solving stiff ordinary differential Equations, NRL Memorandum Report 4091, Naval Research Laboratory, Washington, D.C. (AD-A083 545)

Zabetakis, M.G. (1965) Flammability Characteristics of Combustible Gases and Vapors, U.S. Bureau of Mines Bulletin 627, Pittsburgh, Pa. (AD-701576)

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