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MODELING OF HYDROGEN-AIR DIFFUSION FLAME

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ABSTRACT

Work performed during the first twelve months of the project duration for the NASA Grant (NAG-1-861) is reported here. An analytical and computational study of opposed jet diffusion flame for the purpose of understanding the effects of contaminants in the reactants and thermal diffusion of light species on extinction and reignition of diffusion flames is in progress. The methodologies that have been attempted so far are described. Results using a simple, one-step reaction for the hydrogen-air counterflow diffusion flame are presented. These results show the correct trends in the profiles of chemical species and temperature. The extinction limit can be clearly seen in the plot of temperature vs. Damkohler number.

INTRODUCTION

The laminar, counterflow diffusion flame has become a standard tool for the investigation of stability and extinction characteristics of diffusion flames. In one configuration, the counterflow diffusion flame is obtained in the laboratory by means of flow from two coaxial jets -- fuel from one side and air from the other -- impinging upon each other and forming a stagnation point flow. In a different configuration, air flows towards a porous cylinder from whose surface fuel is injected. These two streams form a stagnation point flow at some distance from the cylinder surface. The two configurations described above have their advantages and disadvantages. From the analysis point of view, both are described by the classical boundary-value problem for stagnation point flow. They differ only in the boundary conditions. The present work describes a procedure for analyzing problems of the boundary-value type. Even though the method is quite general, attention will be focused here on the counterflow difusion flame.

Extinction of the counterflow diffusion flame has been studied extensively because of its importance in predicting blowoff conditions in a practical jet engine. This aspect is becoming increasingly important as new engine concepts such as the supersonic combustion ramjet (SCRAMJET) engine are being developed. A non-dimensional parameter called a Damkohler number is convenient for the study of extinction characteristics of non-premixed flames. We difine a Damkohler number, D_1 , as the ratio of the flow time to chemical reaction time. Therefore, smaller Damkohler numbers represent slower reactions and larger Damkohler numbers indicate faster reactions in relation to the flow time. Extinction and reignition phenomena have been studied with respect to a plot of the flame temperature as a function of the Damkohler number. An S-shaped curve have been obtained for a limited number of cases (Figure 1).

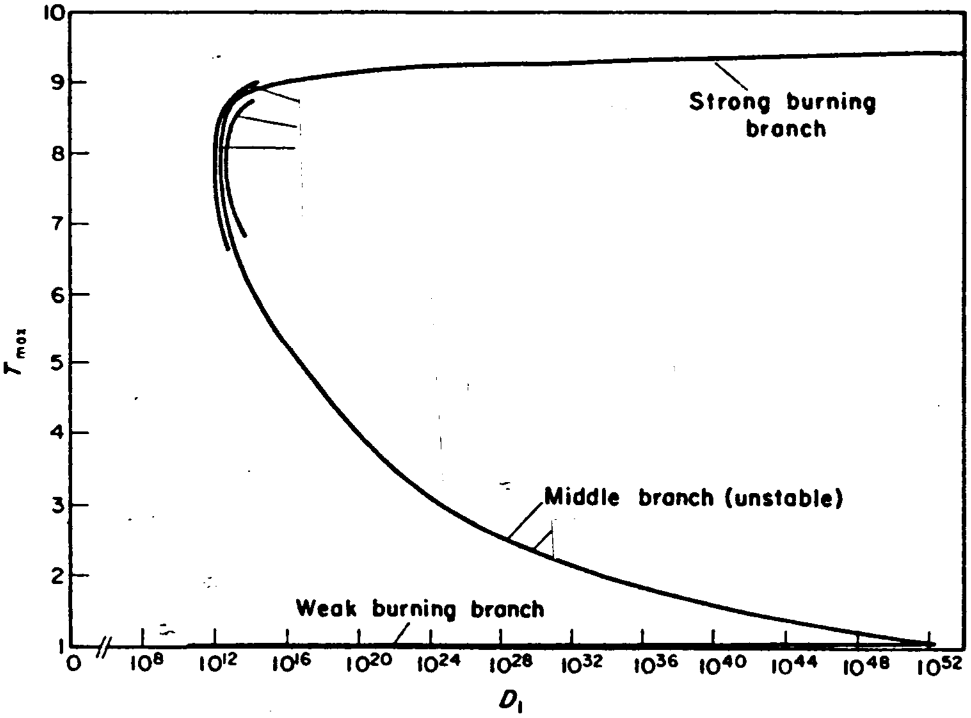

Figure 1. Graphical Representation of Flame Limits

Stability of the flame can be studied with respect to this S-shaped curve. The two vertical tangents at points 1 and 2 represent the extinction and reignition points. The branch A of the curve represents a stable flame; the branch B represents unstable burnig conditions and branch C represents another stable flame. Even though this S-shaped curve have been obtained analytically by asymptotic analysis, the existence of it has not been established by more detailed solution of the governing equations; nor has it been experimentally demonstrated in a universal manner. The motivation for the present study is to conduct a more thorough analysis than has been done before and answer some of the interesting questions that have been raised by the experimental work of Pellet et al[1]. Some of the interesting observations of Pellett and others are decribed in the following paragraph.

An argon-bathed tubular opposed jet burner (OJB) was developed and applied to chemically-limited counterflow diffusion flame, formed by small, (2.7 and 5 mm i.d.) laminar jets hydrogen diluted with nitrogen and air at ambient conditions. Data from pure air as well as air mixed with nitrogen were characterized and used to evaluate similar data for nitric oxide contamination. Two phenomena called 'blowoff' and 'restore' were observed by varying test parameters such as fuel dilution ratio and jet velocity. 'Blowoff' was a sudden breaking of the disk-shaped flame to form a stable torus shape; 'restore' marked the restoration of the flame to the center by radial flame propagation. 'Restore' is a newly discovered flame limit. Both flame limits were sensitive to reactant composition. Blowoff is a measure of flame reactivity and it may be related to a Damkohler number defined as the ratio of flow time to reaction time. 'Restore', on the other hand, appears to be more complex and cannot be explained by flame reactivity alone. The inner edge of the torus-shaped flame is approximately the same diameter as the tubes from which the reactants flow. It is believed that 'restore' is a flame propagation phenomenon: when the fluid velocity at the inner edge of the torus-shaped flame is less than the flame speed, the flame propagates to the central region marking the phenomenon of restore. However, no conclusive evidence is avaialble to back this reasoning. The question that still remains to be answered is whether mixing by diffusion is complete by the time the gases travel outward a distance of one tube diameter. In any case, there is reason to believe that the counterflow flame is a diffusion flame only in the neighborhood of the stagnation point; away from the stagnation point it exhibits some characteristics of premixed flames. Therefore, a simple diffusion flame theory may not be adequate to explain all the phenomena observed in the laboratory.

PRESENT WORK

The present work consists of the solution of the equations governing the fluid flow, conservation of energy and finite rate chemistry for the hydrogen-air counterflow diffusion flame. The equations are reduced to a set of ordinary differential equations by making the classical boundary layer assumptions; they are, therefore, valid only for the stagnation point flow. These equations are of the boundary-value type. The combustion model in the preliminary calculations assumes a one-step forward overall gas-phase chemical reaction of second order occuring in the axisymmetric or two-dimensional stagnation point flow at a solid surface or formed by two opposed jets. The resulting set of equations is as shown below.

$$(C f_{\eta\eta})_\eta + f f_{\eta\eta} + \frac{1}{(1+\epsilon)}\left(\frac{\rho_e}{\rho} - f_\eta^{2}\right) = 0 \qquad (1)$$

$$\left(\frac{C}{P_r} h_\eta\right)_\eta + f h_\eta = 0 \qquad (2)$$

$$\left(\frac{C}{P_r} L_{eF} Y_{F\eta}\right)_\eta + f Y_{F\eta} + \frac{1}{2a}\frac{\dot{w}'''}{\rho} = 0 \qquad (3)$$

The chemical reaction rate for the one-step second order reaction is given by

$$\dot{w}''' = Z_a \rho^2 Y_F Y_O \exp\left(-E_a / \bar{R} T\right) \qquad (4)$$

in which w is mass of fuel consumed per unit volume per unit time. Define the first Damkohler number as

$$D = Z_a \rho / a(1+\alpha)$$

Introducing Eq. (5) into Eq. (3), the species conservation equation becomes

$$\left(\frac{C}{P_r} L_{eF} Y_{F\eta}\right)_\eta + f Y_{F\eta} + D Y_F Y_O \exp\left(-E_a / \bar{R} T\right) = 0 \qquad (5)$$

Boundary Conditions

The appropriate boundary conditions have to be applied depending on the geometry of the problem. For the opposed jet problem the boundary condtions are given as

$$\eta = -\infty$$

$$f_\eta(-\infty) = \frac{U_{-\infty}}{U_\infty}$$

$$h(-\infty) = \left(h_{H_2} Y_{H_2} + h_{N_2} Y_{N_2}\right)_{-\infty}$$

$$Y_F(-\infty) = Y_{F\,-\infty}$$

$\eta = 0$ $\quad f = 0$

$\eta = \infty$

$$f_\eta(\infty) = 1$$

$$h(\infty) = (h_{O_2} Y_{O_2} + h_{N_2} Y_{N_2})_\infty$$

$$Y_F(\infty) = 0$$

For the stagnation point flow over a surface one can write the boundary conditions as

$\eta = 0$

$$f_\eta(0) = 0$$

$$f(0) = f_N$$

$$h(0) = (h_F Y_F + h_{N_2} Y_{N_2})_0$$

$$Y_F' = S_c f_w (1 - Y_{Fw})$$

$\eta = \infty$

$$f_\eta = 1$$

$$h(\infty) = (h_O Y_O + h_{N_2} Y_{N_2})_\infty$$

$$Y_F(\infty) = 0$$

NUMERICAL SOLUTION

Several different numerical approaches have been attempted; some of them proved to be more suitable for the present problem than the others. The main difficulty in the solution procedure stems from the fact that the equations become stiff as the number of chemical reactions increase. Stiffness is defined as the condition where the eigenvalues of the Jacobian Matrix of the locally linearized representation of the equation set have negative real parts that fall over a large range; eigenvalues differing by 5 or 6 orders of magnitude are common in chemically reacting flow problems. Stiffness limits the choice of step size that can be used for the numerical integration of the problem; as a result computation time becomes prohibitive. Several techniques are in use to circumvent the difficulties associated with the solution of stiff equations. Multistep methods such as used in the widely used routines like LSODE [2] are useful for solving initial value problems in ordinary differential equations. No such well proven methods are available for boundary value problems in ordinary differntial equations or for solving stiff partial differential equations. The present work is based, therefore, on methods chosen by intuition rather than any well established criteria.

Numerical algorithms for the governing equations described earlier have been developed and they have been implemented on the NASA Langley computer system as well as the computer system at the University of Missouri-Rolla. The following are brief descriptions of the algorithms.

1. Collocation Method: This is a routine called COLSYS [3] available from the Langley Math Library. The routine can be used to solve boundary-value problems governed by a system of ordinary differential equations.

2. Fully Implicit Finite Difference Method: Recognizing the stiff nature of the differential equations because of the presence of the chemical

source term, a fully implicit algorithm was written to avoid the limitation on step size for stable solution.

3. Patankar and Spalding Method: This method uses the conservative form of the equations. The source term is treated according to the rules formulated by Patankar[4].

Work in Progress

The method that has been used for the results given in this report is a combination of COLSYS for the solution of the fluid dynamic equation and the fully implicit method for the solution of the energy equation and the species continuity equation. The COLSYS routine has been found to be well suited for the solution of the fluid dynamic equation which is third order. Also it is well recognized that, for this case, the fluid dynamic equation is only weakly coupled with the energy and the species continuity equations. Therefore, the fluid dynamic equation is solved first with assumed initial profiles. With the values of the similarity variable f and its derivatives obtained from the solution by COLSYS, the energy equation and the species continuity equations are solved simultaneously by using the fully implicit solution procedure. The grid spacing in the eta direction and the time step are both variable. The grid spacing in the eta direction is chosen such that they are closely spaced in the region where the temperature and the species mass fractions have high gradients. The time step is varied in an ad hoc manner so as to reduce computation time and to preserve time accuracy of the solution.

PRELIMINARY RESULTS

Some preliminary results of the calculations are shown in Figures 1 -5. These are preliminary results and therefore, their numerical values are not to be stressed. It was found that the results depend on factors such as the grid spacing. A grid independent solution should, therefore, be obtained by further refining the grid. A course grid is presently used to reduce computer run time. Variable time step was used to decrease the time required to reach asymptotic values. The results shown are the values obtained at the end of 3000 time steps. It was observed that slight oscillations of the solutions persist even at this stage; however, these were observed to be too small to have any significant effect on the solution. The CPU time required for these runs is approximately 50 minutes on the IBM 4381 mainframe computer.

Figures 1, 2 and 3 are for the hydrogen-air case. Figure 1 shows the temperature profile for one value of the velocity gradient. The peak temperature of 3300 K is higher than the adiabatic flame temperature because these values are based on constant specific heat assumption. Subsequent runs with variable specific heats have shown that the peak temperature is lower than the adiabatic flame temperature. Two other temperature profiles corresponding to extinction conditions are also shown in the plot.

Figures 2 shows the corresponding mass fraction profiles. These profiles agree in shape with published data. It can be seen that hydrogen and oxygen concentrations go to zero at the flame zone. Water exists in significant amounts over a wider region to either side of the flame zone.

Figure 3 shows the extinction conditions. As the Damkohler number decreases the maximum temperature decreases; the vertical portion of this curve may be thought of as the extinction condition. Again, it must be emphasized that the numerical values are quite different from previously published numbers because the values of the frequency factor and the activation energy used in the calculations were not realistic; subsequent calculations show extinction strain rates much closer to experimentally observed values.

Figures 4 and 5 show results for a carbon monoxide-air flame. The trends are similar to the hydrogen-air flame. As expected, the peak temperature is lower for this case.

WORK IN PROGRESS

The following is a list of cases that are being run presently.

1. Opposed jet case.
2. Effect of activation energy and frequency factor on extinction.
3. Effect of time step size on the solution.
4. Effect of grid spacing in the eta direction.
5. Runs to compare the strain rate vs. fuel mole fraction for extinction curve of Pellet et al.

REFERENCES

1. Pellett, G. L., Northam, G. B., Guerra, R., and Wilson, L. G., " Opposed Jet Burner Studies of Silane-Methane, Silane-Hydrogen and Hydrogen Diffusion Flame with Air," 23rd JANNAF Combustion Meeting, October 20-24, 1986, Hampton, VA.

2. Hindmarsh, A., "LSODE..Livermore Solver of Ordinary Differential Equations," 1980.

3. Asher, U., Christiansen, J and Russell, R. D., "COLSYS: Collocation Software for Boundary-Value ODEs, ACM Trans. on Math. Software, Vol.7.

4. Patankar, S. V., <u>Numerical Heat Transfer and Fluid Flow</u>, Hemisphere, Washington, D.C., 1980.

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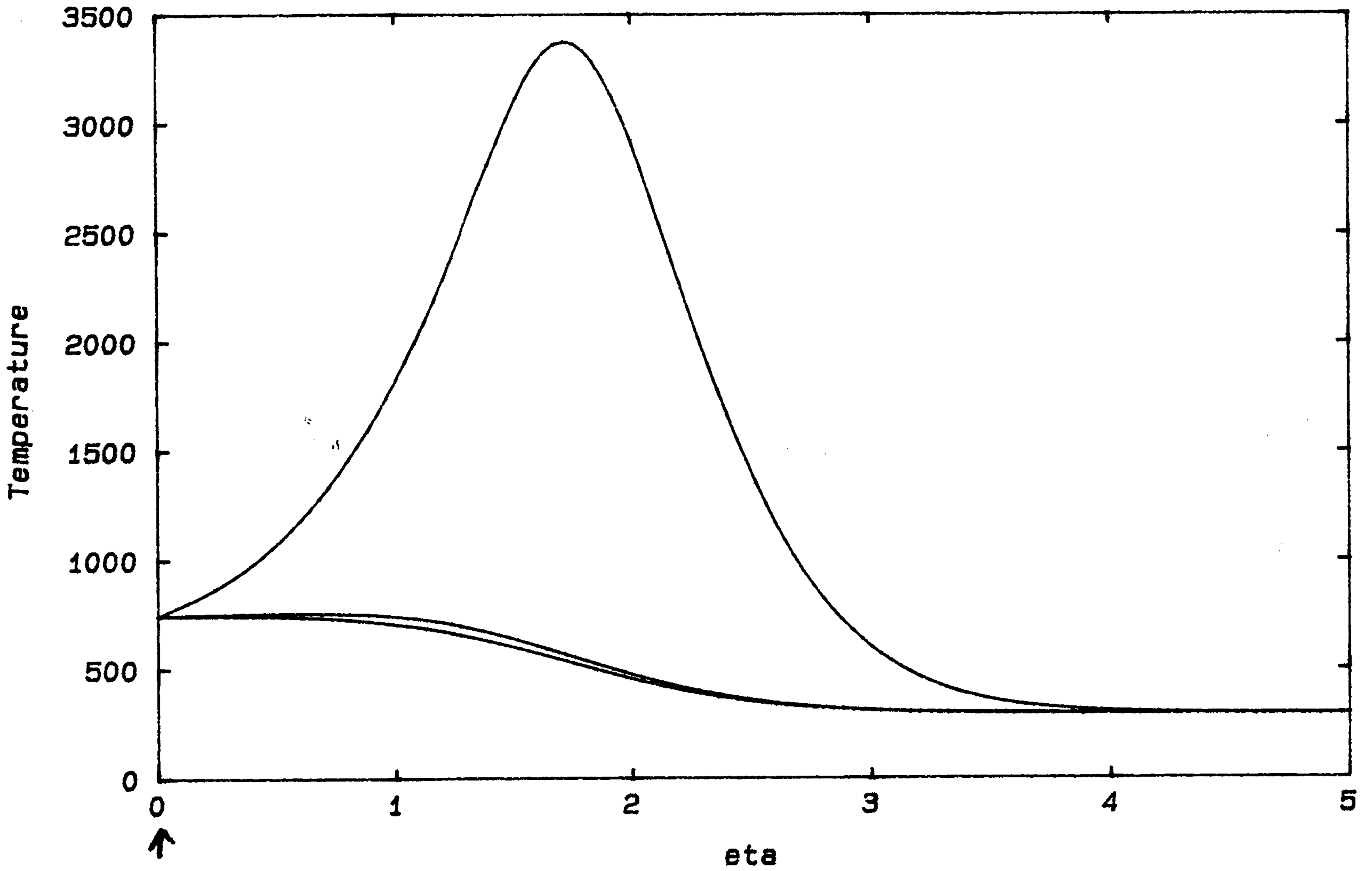

Sphere surface

Fig. 1 Temperature Distribution

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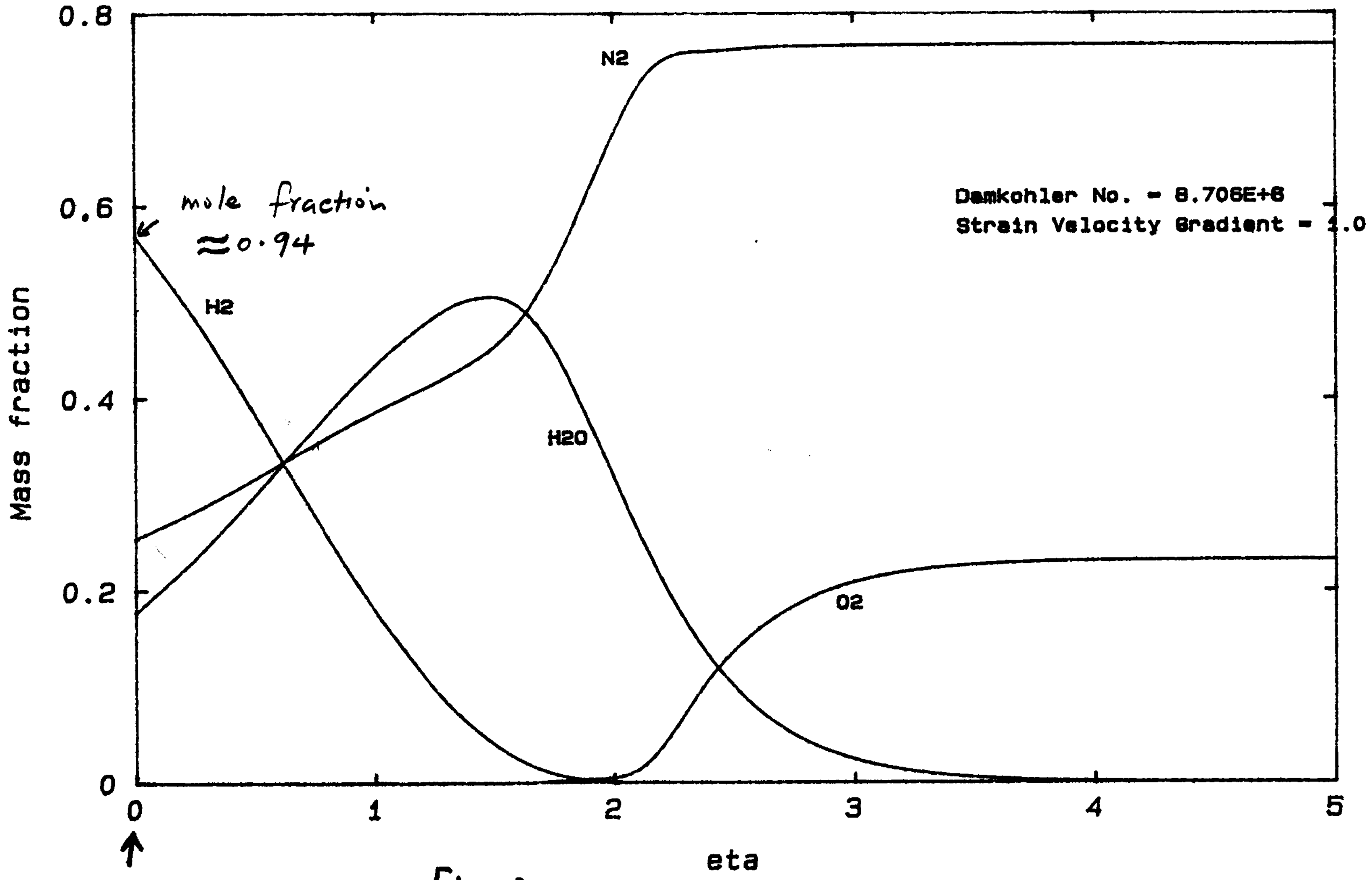

mole fraction
≈ 0.94

↑
Sphere surface

Fig. 2
Species Mass Fraction Distribution

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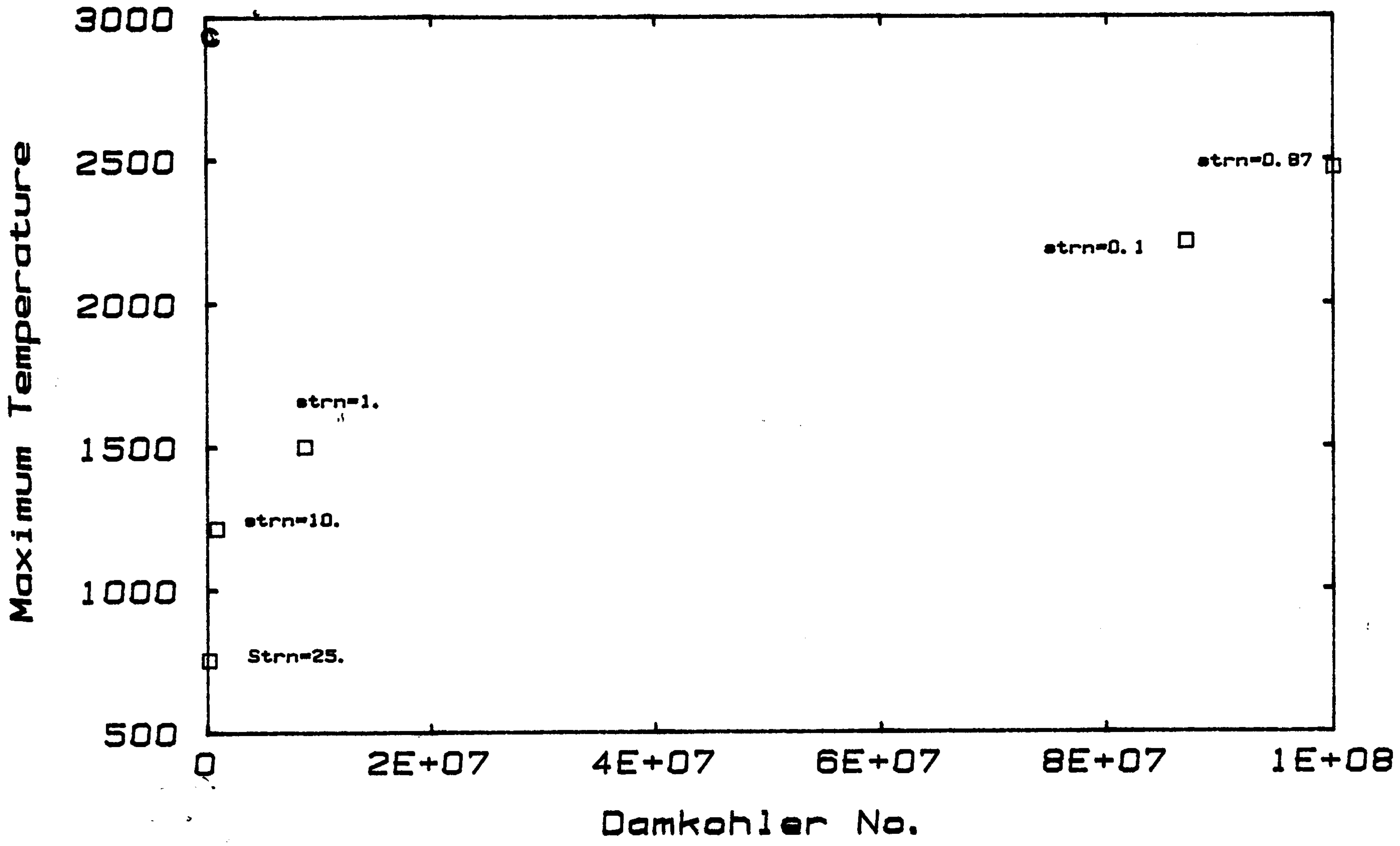

Fig. 3 Maximum Temperature vs Damkohler No.

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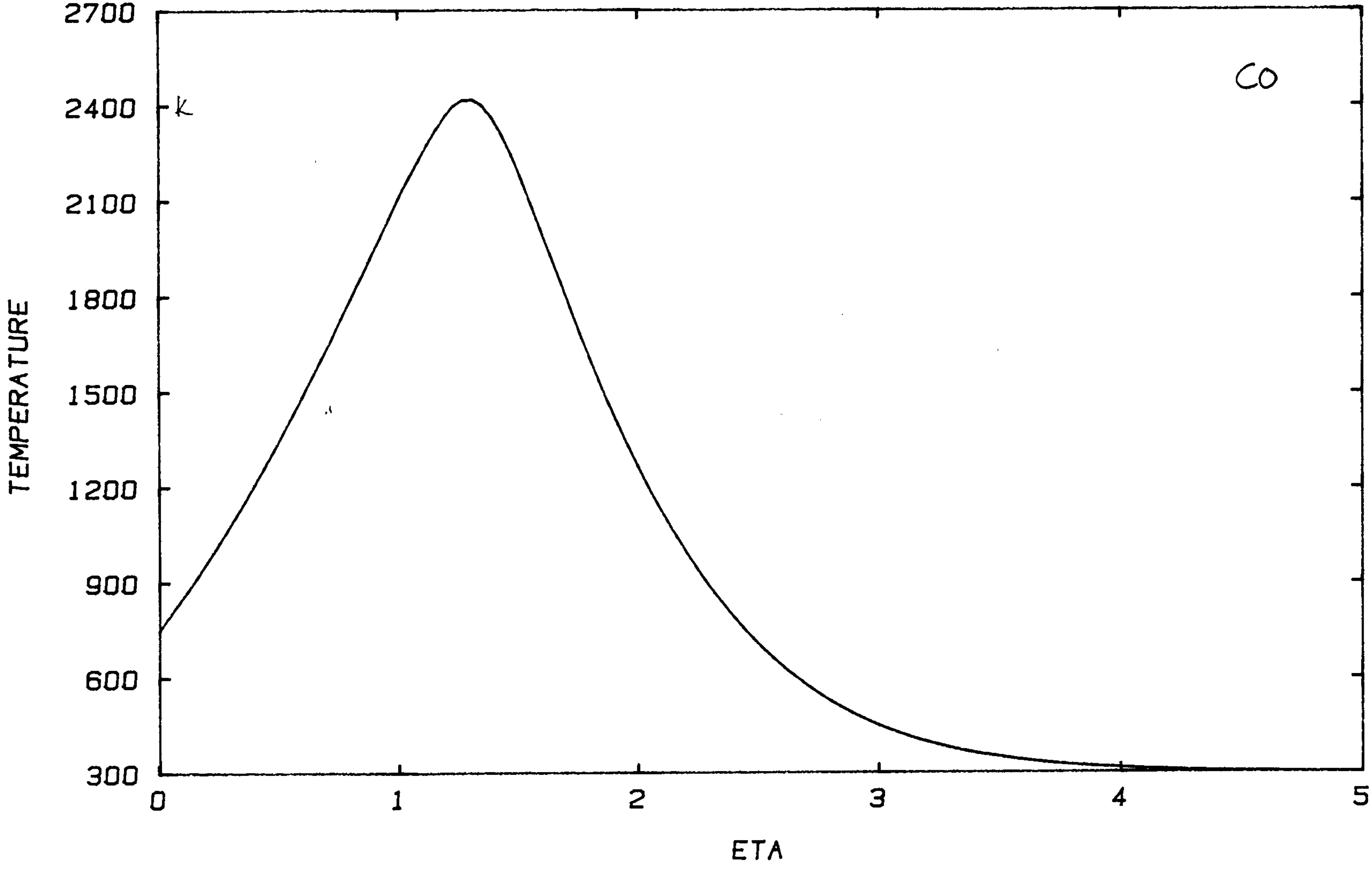

Fig. 4 TEMPERATURE PROFILE

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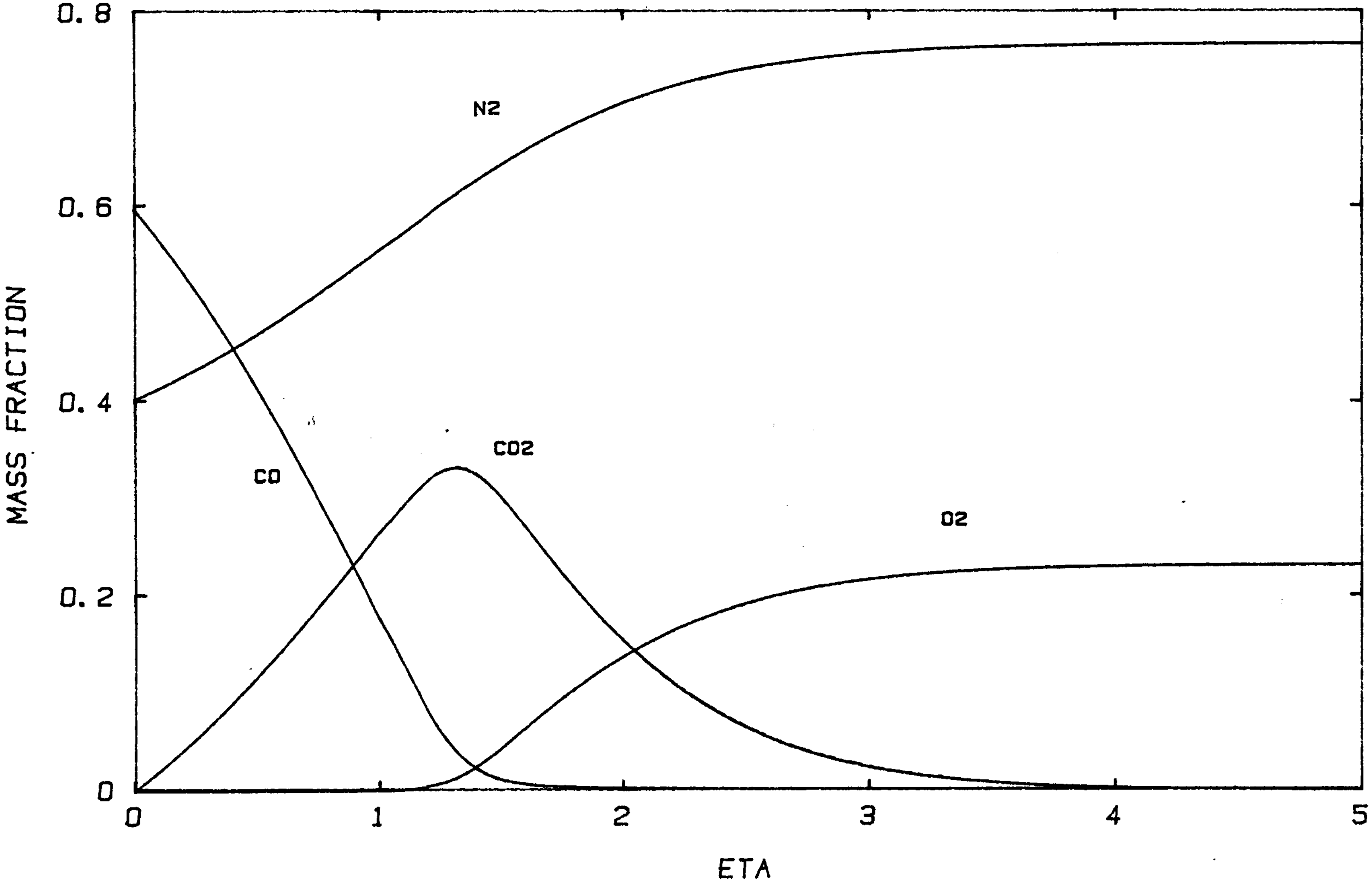

Fig. 5 SPECIES PROFILES