Using a Global Hydrogen-Air Combustion Model in Turbulent Reacting Flow Calculations

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A two-step global model describing the combustion of hydrogen in air at 1 atm pressure is developed by comparing the temperature histories obtained from a 28 reaction H-O mechanism. Using criteria discussed herein, good agreement is obtained in the range of initial mixture temperatures of 1000-2000 K and in the range of equivalence ratios of 0.2-2.0. The two-step global model is compared with the results obtained using an eight-step, H-O reaction mechanism in a computer program describing the turbulent diffusion of hydrogen in supersonic axisymmetric and two-dimensional reacting flows. Comparisons of profiles of temperature and pitot pressure are presented. The global model is judged to be adequate in flows which are not dominated by long ignition delay times.

Introduction

THE numerical calculation of the turbulent mixing and reaction of fuel in the supersonic flow through a scramjet combustor is a computational problem of considerable interest. In addition to the usual complexities involved in numerical integration of the parabolic Navier-Stokes equations, it is often necessary to include details of the finite-rate chemical kinetics of the fuel-air reactions. The introduction of detailed chemical reaction mechanisms into theoretical analyses of complex turbulent mixing flows often results in excessive computer run times and storage requirements. The simplification of the chemistry mechanism to a few essential reactions that model, to reasonable accuracy, the overall nature of the reaction is desirable.

A number of simplifications have been employed in an effort to realize this goal and, thereby, to avoid the difficulties of long computer run times and large storage requirements. One such attempt has been to assume that chemical reaction occurs by means of an arbitrarily postulated, one-step, irreversible reaction. If it is also assumed that this reaction occurs very rapidly, the problem reduces to one in which the rate of combustion is entirely mixing controlled (see, for example, Refs. 1 and 2). A related concept involves the assumption that the fuel and oxidizer react instantaneously and form reaction products in chemical equilibrium.[3] Such "fast chemistry" assumptions are valid only for high-temperature, mixing controlled diffusion flames involving rapidly reacting components.

A less restrictive approximation of a multireaction chemical kinetic mechanism is to assume that all two-body "shuffle" reactions occur so quickly under all conditions that they are in equilibrium at all times; only the rate-limiting three-body recombination reactions are treated kinetically. Such an approach was employed for a seven-reaction chemical kinetic mechanism for hydrogen-air combustion in Ref. 4. This "partial equilibrium" assumption is limited in applicability to high temperatures (>1200 K), pressures near 1 atm, and fuel oxidizer mixtures near stoichiometric.[4] A similar approach for the oxidation of propane assumed an infinitely fast reaction to form CO and an equilibrium mixture of H-O species.[5] The subsequent oxidation of CO and all three-body reactions involving H-O species proceeded at a finite rate. Two-body H-O reactions, however, were assumed to be in chemical equilibrium. As in Ref. 4, these assumptions apply only to high-temperature, stoichiometric flames near atmospheric pressure.

Apparently, the first attempt at formulating a simplified, finite-rate combustion mechanism for use in multidimensional flame analyses was that of Edelman and Fortune.[6] In this work, a hydrocarbon-air reaction mechanism involving 69 reactions of 31 species from Ref. 7 was reduced to a "quasiglobal" mechanism. The quasiglobal model consisted of an initial finite-rate step, wherein the hydrocarbon fuel was partially oxidized to CO and H_2, followed by nine elementary kinetic reactions by which CO and H_2 were oxidized. Thus, the chemistry was effectively reduced to a 10-reaction mechanism. Although this resulted in an appreciable reduction in computer running times compared with the 69-reaction mechanism it is, nonetheless, a kinetics mechanism of substantial size.

Recent research has led to the formulation of global and quasiglobal models for CO and hydrocarbon fuels.[8-10] In Ref. 8, a global model was experimentally deduced for moist CO oxidation and reference is made to a global expression for methane oxidation. Further work resulted in models for ethane and ethene[9] and, most recently, to a proposed four-step global model for the oxidation of any alkane hydrocarbon.[10] However, these models have not been evaluated in multidimensional flame analyses.

In this paper, we propose a two-step global model for H_2 combustion. The proposed model was deduced from results obtained with a 28-reaction mechanism employed in a series of one-dimensional, constant-pressure, stream-tube calculations. The global model was then used in calculations describing the two-dimensional, turbulent mixing and combustion of H_2 in a supersonic flow of air at 1 atm pressure. Results of these calculations in the form of temperature and pitot pressure profiles and distributions of mixing and heat release are compared with similar results for

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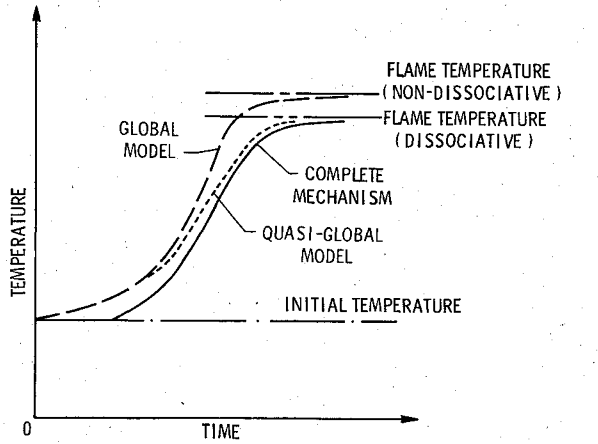


Fig. 1 Schematic illustrating the general behavior of chemical kinetic mechanisms.

an eight-reaction H_2-O_2 kinetics mechanism. This eight-reaction mechanism had previously been shown to compare well with two sets of experimental data.[11]

Development of the Global Model

Alleviating excessive computer run times and storage problems by the reduction of a complete chemical kinetics mechanism to a few reactions will, of course, have limitations. In particular, two such limitations of a global model should be noted:

1) During the ignition delay period, when the complete mechanism will predict the gradual buildup of free radicals with little or no perceptible temperature change, a global model will indicate an immediate exothermic or endothermic reaction with attendant temperature increase or decrease, respectively. This change in temperature is schematically illustrated in Fig. 1. Hence, one criterion for a successful global model is that this initial temperature change be held to a minimum so that the ignition delay period is adequately represented. For flow situations involving very long ignition delays, this may be difficult to accomplish.

2) The adiabatic flame temperature for the global model will be higher than for the complete mechanism. This higher temperature results from the fact that a global model does not include all of the product species actually present at equilibrium; hence, it will predict a non-dissociative or, at best, partially dissociative flame temperature as illustrated in Fig. 1. One approach to eliminating this limitation is to use a "quasiglobal" mechanism[6] wherein the initial reactants are taken through a partial oxidation to intermediate species which are then oxidized to completion via a multireaction mechanism (Fig. 1). Although this approach may reduce the number of elementary reactions to eight or ten, it is still quite large for parametric calculations of diffusion flames. The principal computational benefits to be achieved by the global-modeling approach stem from reducing, to the greatest extent possible, the size of the original mechanism. Hence, some sacrifice in flame temperature accuracy is deemed warranted. If very low pressures are avoided, the discrepancy in the flame temperatures will not be sufficient to merit concern in the majority of analyses employing these models.

The principal criterion used herein to develop the global model and its associated reaction rate constants was its ability to replicate the temperature history of the complete mechanism over the range of conditions of interest. This point is schematically illustrated in Fig. 2 where a typical temperature history, obtained from a constant-pressure stream-tube analysis using a complete mechanism, is compared with the results that might be obtained from two typical global models. Although global model 1 more accurately estimates the ignition delay time t_{ig}, it would be rejected because of overall poor comparison with the actual temperature history. Global model 2, however, is considered to be acceptably accurate in reproducing the temperature history of the complete mechanism.

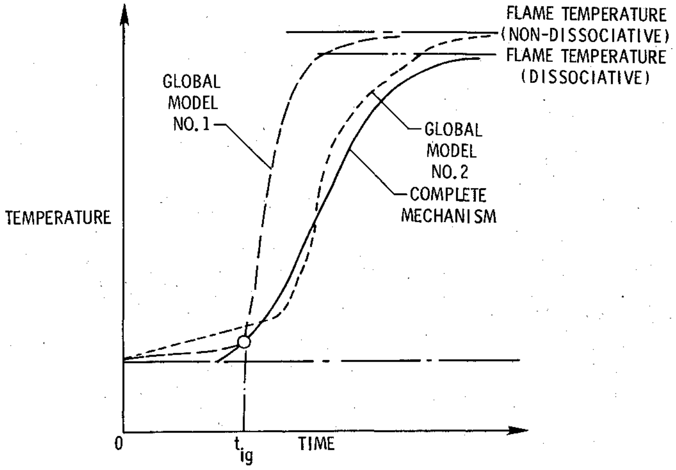


Fig. 2 Schematic comparing global models with a complete mechanism.

From these considerations, the importance of the form required for a global model was deduced. It was found that, in general, the following types of reactions are required:

$$F+O=I(+S) \tag{1}$$

$$I+O=P(+S) \tag{2}$$

$$(S+O=P) \tag{3}$$

where F = fuel, O = oxidizer, I = an intermediate species (generally a free radical), S = a stable intermediate, and P = product species. The parentheses indicate that species S or reaction (3) may or may not be present. The key to developing an acceptable global model within the stated criteria is the selection of the intermediate species I. The importance of selecting the appropriate intermediate species also was concluded independently by Hautman et al.[10] Reaction (1) controls the reaction of the fuel and oxidizer species through the ignition delay period, whereas reaction (2) predominates during the combustion phase when the major heat release and product formation occurs. As a result, reaction (2) must be sufficiently exothermic to insure that the principal temperature increase occurs as a consequence of that reaction.

Application of the considerations discussed above leads to the following proposed two-step global model for the oxidation of hydrogen in oxygen at 1 atm:

$$H_2 + O_2 \overset{k_{f4}}{\rightleftarrows} 2OH \tag{4}$$

$$2OH + H_2 \overset{k_{f5}}{\rightleftarrows} 2H_2O \tag{5}$$

with the forward reaction rate constants given in the form of an Arrhenius equation

$$k_{fi} = A_i(\phi)\, T^{N_i} \exp(-E_i/RT) \tag{6}$$

where the pre-exponential $A_i(\phi)$ is a function of equivalence ratio. The values of the parameters $A_i(\phi)$, N_i, and E_i in Eq. (6) were determined for reactions (4) and (5) by comparison of temperature histories in a constant-pressure stream-tube reactor. Values of the parameters were established for

Table 1 Hydrogen-oxidation chemical kinetic mechanism[a]

Reaction No.	Reaction	Reaction rate variables[b] *A*	*N*	*E*
1[c]	$M + O_2 = O + O$	0.72000E+19	−1.0000	117,908
2[c]	$M + H_2 = H + H$	0.55000E+19	−1.0000	103,298
3[c]	$M + H_2O = H + OH$	0.52000E+22	−1.5000	118,000
4	$H + O_2 = HO_2 + M$	0.23000E+16	0.0000	−800
5	$M + H_2O_2 = OH + OH$	0.12000E+18	0.0000	45,500
6	$M + O_3 = O_2 + O$	0.13000E+22	−2.0000	25,433
7[c]	$O + H = OH + M$	0.71000E+19	−1.0000	0
8[c]	$H_2O + O = OH + OH$	0.58000E+14	0.0000	18,000
9[c]	$H_2 + OH = H_2O + H$	0.20000E+14	0.0000	5,166
10[c]	$O_2 + H = OH + O$	0.22000E+15	0.0000	16,800
11[c]	$H_2 + O = OH + H$	0.75000E+14	0.0000	11,099
12	$H_2 + O_2 = OH + OH$	0.10000E+14	0.0000	43,000
13	$H + HO_2 = H_2 + O_2$	0.24000E+14	0.0000	695
14	$H_2 + O_2 = H_2O + O$	0.41000E+14	0.0000	50,470
15	$H + HO_2 = OH + OH$	0.24000E+15	0.0000	1,887
16	$H_2O + O = H + HO_2$	0.58000E+12	0.5000	57,000
17	$O + HO_2 = OH + O_2$	0.50000E+14	0.0000	1,000
18	$OH + HO_2 = O_2 + H_2O$	0.30000E+14	0.0000	0
19	$H_2 + HO_2 = H_2O + OH$	0.20000E+14	0.0000	25,000
20	$H + H_2 = H + H_2O_2$	0.73000E+12	0.0000	18,677
21	$H_2O_2 + H = OH + H_2O$	0.32000E+15	0.0000	8,950
22	$HO_2 + OH = O + H_2O_2$	0.52000E+11	0.5000	21,062
23	$HO_2 + H_2O = OH + H_2O_2$	0.28000E+14	0.0000	32,785
24	$HO_2 + HO_2 = H_2O_2 + O_2$	0.20000E+13	0.0000	0
25	$O + O_3 = O_2 + O_2$	0.10000E+14	0.0000	4,790
26	$O_3 + H = O_2 + O_2$	0.70000E+14	0.0000	1,113
27	$O_3 + OH = HO_2 + HO_2$	0.90000E+12	0.0000	1,987
28	$O_3 + HO_2 = O_2 + OH$	0.10000E+12	0.0000	2,800

[a] Taken from Ref. 12. [b] Form of rate constant is $k = AT^N \exp(-E/RT)$ with k in $cm^3 \cdot mole^{-1} \cdot s^{-1}$ and E in $cal \cdot mole^{-1}$. [c] Reactions of eight-reaction mechanism of Ref. 11.

reaction (4) as

$$A_4(\phi) = (8.917\phi + 31.433/\phi - 28.950) \times 10^{47},\ cm^3/mole \cdot s$$

$$E_4 = 4865\ cal/mole \tag{7}$$

$$N_4 = -10$$

and reaction (5) as

$$A_5(\phi) = (2.000 + 1.333/\phi - 0.833\phi) \times 10^{64},\ cm^6/mole^2 \cdot s$$

$$E_5 = 42{,}500\ cal/mole \tag{8}$$

$$N_5 = -13$$

for initial temperatures of 1000-2000 K and equivalence ratios of 0.2-2.0. With these values, the temperature histories given by the global model adequately reproduced those of the 28-reaction mechanism given in Table 1. These 28 reactions were taken from the full 60-reaction H_2-air mechanism used in the study of hydrogen ignition and reaction reported in Ref. 12.

Comparisons of the temperature histories of the global model and the 28-reaction mechanism for $\phi = 1.0$ are presented in Fig. 3. For each initial temperature the results for the global model (broken lines) are slightly higher than for the 28-reaction mechanism (solid lines), which is denoted as "full mechanism" in the figure. However, the shapes of the temperature histories are accurately represented.

The need for an equivalence ratio correction to the pre-exponential parameters can be seen from the temperature history comparisons for $\phi = 2.0$ in Fig. 4. The results obtained with the global model using the $\phi = 1.0$ values of A_4 and A_5 are labeled "global, no ϕ correction" in the figures, and inadequately follow the 28-reaction (full mechanism) results. By adjusting the values of the pre-exponential parameters, the global model gave results shown by the lines labeled "global, with ϕ correction." These results more accurately duplicate

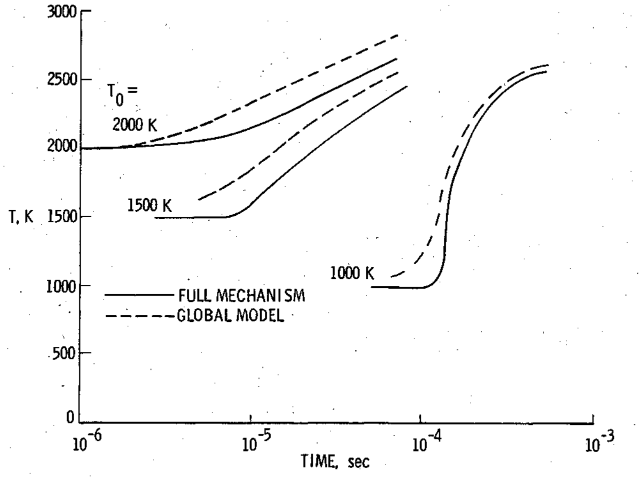


Fig. 3 Temperature histories for H_2-air at 1 atm ($\phi = 1.0$).

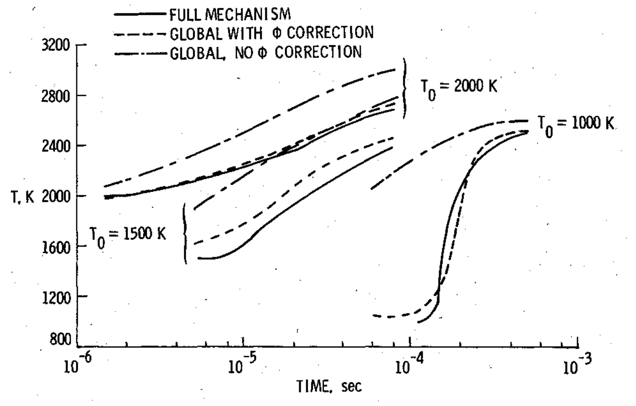


Fig. 4 Temperature histories for H_2-air at 1 atm ($\phi = 2.0$).

those of the 28-reaction (full) mechanism over the temperature range. Similarly, the pre-exponentials for the $\phi = 0.2$ mixture were adjusted in value to give comparable results with the full mechanism. The functions for the ϕ-dependence of the pre-exponentials given by Eqs. (7) and (8) were obtained by curve fitting the three values of A_4 and A_5 for equivalence ratios of 0.2, 1.0, and 2.0.

From the comparisons presented in Figs. 3 and 4 it is concluded that the global model should be adequate for the calculation of hydrogen reacting in air in a constant pressure (1 atm) steam tube at conditions of temperature and equivalence ratio within the ranges indicated.

Application of the Global Model

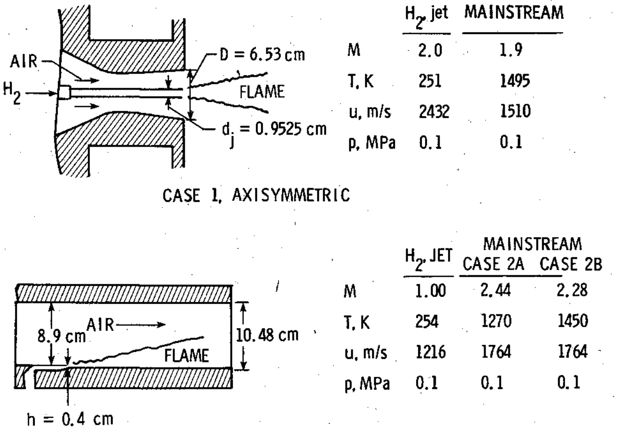
Having established the two-step global model, an investigation was conducted to determine its ability to model the chemistry in calculations of turbulent mixing and reacting flowfields. In these calculations, the present global model is tested against a more exact chemistry mechanism. The test cases are the same as those from Ref. 11 in which experimental data were successfully predicted by both 8- and 25-reaction chemical kinetic mechanisms. For the purposes of testing the global model, the eight-reaction mechanism (denoted by ( )^c in Table 1) was considered to be sufficient.

Description of Test Cases

The two cases chosen for the application of the global model to diffusion flames are illustrated in Fig. 5. Case 1 is an axisymmetric flow with a central Mach 2 hydrogen jet at a static temperature of 251 K within a Mach 1.9 air mainstream at a static temperature of 1495 K. Nominal static pressure of both the jet and mainstream is 1 atm. Case 2 is for a two-dimensional flow with a sonic hydrogen jet at a static temperature of 254 K issuing parallel along one wall. The results presented in Ref. 11 were for case 2A with the Mach 2.44 mainstream air at the 1270 K static temperature of the experimental tests. Because of the low static temperature, this case had a significantly long ignition delay time. To investigate the effect of this lower temperature, a case 2B was run with a mainstream temperature of 1450 K. The jet and mainstream are both at 1 atm pressure. These cases provide a means of checking the global model for different geometries and initial conditions.

Computer Program

The computer program used for the comparative calculations is a two-dimensional, parabolic flow code that uses the finite difference technique of Pantankar and Spalding[13] to solve the parabolic partial differential equations for the transport of momentum, energy, and mass. The code employs the so-called k-ϵ two-dimensional model of turbulence in which the effective turbulent viscosity is obtained from the turbulent kinetic energy and the dissipation rate of turbulence kinetic energy. The program may be applied to either a two-dimensional or axisymmetric geometry. Additional details of the computer code, and the transport equations are given in Ref. 11.



	H_2 jet	MAINSTREAM
M	2.0	1.9
T, K	251	1495
u, m/s	2432	1510
p, MPa	0.1	0.1

	H_2 JET	MAINSTREAM CASE 2A	MAINSTREAM CASE 2B
M	1.00	2.44	2.28
T, K	254	1270	1450
u, m/s	1216	1764	1764
p, MPa	0.1	0.1	0.1

Fig. 5 Geometry and initial conditions of the test cases.

Use of the Two-Step Global Model

In order to insert the present global model, defined by reactions (4) and (5) and Eqs. (6-8), into the computer code it was first necessary to obtain reaction rates for the reactions in the backward direction. The backward rates were obtained by imposing the requirement that the equilibrium constant $K = k_f/k_b$.

The first attempts at computing the flowfield of the test cases using the global model failed computationally. Examination of the code output revealed the problem to be the large instantaneous rate of production of the hydroxyl radical $\dot{M}_{OH}$. The magnitude of $\dot{M}_{OH}$, which is the source term in the equation for the turbulent transport of OH, was so large that across one computation step, concentrations greater than one were obtained. For other species (H_2,O_2), negative concentrations occurred. It is not unusual in problems involving finite-rate chemical kinetics, that the production rates of several species will become so large that a realistic solution cannot be obtained across one computational step. This solution failure usually manifests itself in one of the above ways. The usual procedure for handling this difficulty is to reduce the step size and, thereby, refine the integration. The use of smaller steps may, however, nullify the advantage of a global model to reduce computation time and costs.

To further assess this problem, the magnitude of the rates of production of each of the four species in the global model were examined. The production rates are

$$\dot{M}_{O_2} = k_{f4} C_{H_2} C_{O_2} + k_{b4} C_{OH}^2 \tag{9}$$

$$\dot{M}_{H_2O} = 2(k_{f5} C_{OH}^2 C_{H_2} - k_{b5} C_{H_2O}^2) \tag{10}$$

and

$$\dot{M}_{H_2} = \dot{M}_{O_2} - ½\dot{M}_{H_2O} \tag{11}$$

$$\dot{M}_{OH} = -(2\dot{M}_{O_2} + \dot{M}_{H_2O}) \tag{12}$$

where the C_i are species concentrations in mole/cm^3. Numerical integration of these equations with time over a time interval corresponding to the computational step revealed that the reaction $H_2 + O_2 = 2OH$ goes to equilibrium very quickly. The result of this numerical integration is illustrated schematically in Fig. 6. The mass fraction history of OH in Fig. 6 rises rapidly until a time that is typically on the order of 10^{-10} s. At this point the rate of production of

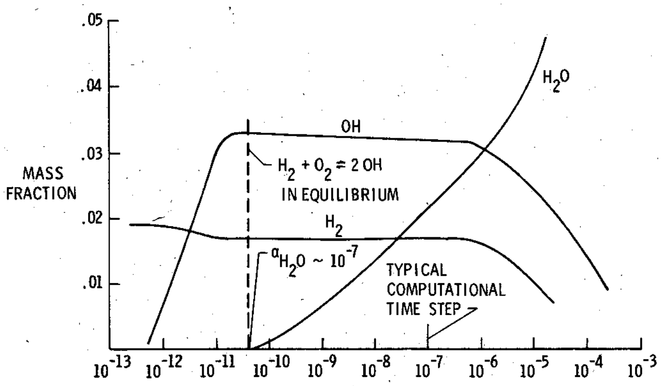


Fig. 6 Schematic of species mass fraction history for global model.

OH is near zero and the OH formation reaction is essentially in equilibrium. The amount of water produced at this point is typically a mass fraction of about 10^{-7}. In the computer program, a typical computation step is about 10^{-4} m which, for a local velocity on the order of 10^3 m/s, corresponds to a time on the order of 10^{-7} s. Therefore, reaction (4) may be in chemical equilibrium during much of the time required for a typical computational step.

In order to alleviate the computational problems caused by the excessively large initial rates of production, a procedure was formulated to determine mean values of the production rates of each species over each computation time step of the computer program. The procedure was to numerically integrate Eqs. (9-12) over a time interval corresponding to the computational step size and the local velocity. The mean rate of production of each species over the computational step was the change in the concentration of that species divided by the computational time step. During the integration when the magnitude of the instantaneous rate of production of OH became small, the reaction was assumed to be in equilibrium. Typically, as indicated in Fig. 6, this event occurred in three or four orders of magnitude less time than the computation step. At the equilibrium point, the concentrations of OH, H_2, and O_2 are related by the law of mass action

$$C_{OH}^2 = K C_{H_2} C_{O_2} \tag{13}$$

where K is the equilibrium constant of reaction (4). By conservation of mass, the concentration of H_2 and O_2 are

$$C_{H_2} = F_H - C_{H_2O} - \tfrac{1}{2} C_{OH} \tag{14}$$

$$C_{O_2} = F_O - \tfrac{1}{2} C_{OH} - \tfrac{1}{2} C_{H_2O} \tag{15}$$

where F_H and F_O are the total amounts of hydrogen and oxygen present in any form. Substitution of Eqs. (14) and (15) into Eq. (13) gives

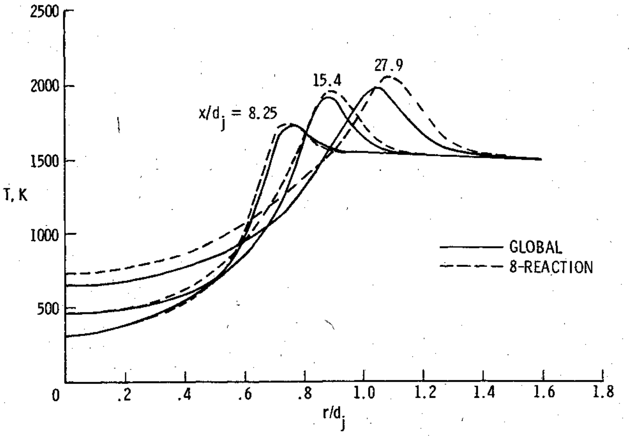
$$\left(\frac{1}{K} - \tfrac{1}{4}\right) C_{OH}^2 + \left[\tfrac{1}{2}(F_H + F_O) - \tfrac{3}{4} C_{H_2O}\right] C_{OH}$$

$$+ \left(\tfrac{1}{2} F_H + F_O\right) C_{H_2O} - \tfrac{1}{2} C_{H_2O}^2 - F_H F_O = 0 \tag{16}$$

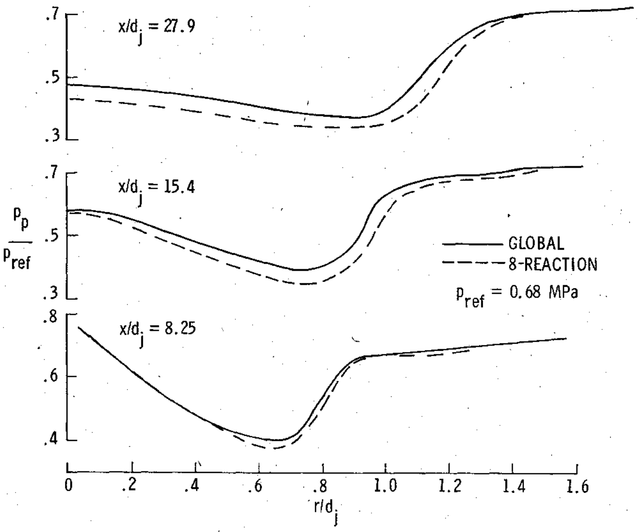
The solution of Eq. (16) relates C_{OH} to C_{H_2O}, which is determined by numerical integration of Eq. (10). When the total integration time equals the time of the computational step, the integration stops, the mean rates of production are computed, and the computer code proceeds with the parabolic flow solution. It should be noted that the assumption of equilibrium would not be imposed in the event that the computational time step is less than the time for the rate of production of OH to become small.

Discussion of Comparisons and Results

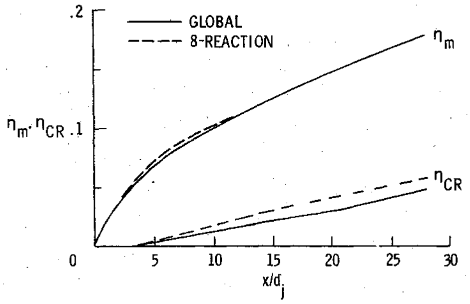
The results obtained using the two-step global model in the computation of turbulent flow with mixing and reaction for the two cases are presented in this section. Based on the previous discussion, the global model should not be expected to reproduce exact profiles of chemical species nor should it necessarily model the ignition phase. Rather, the results obtained with the global model should be representative of the overall flowfield with regard to the mixing of the fuel and the overall heat release. Therefore, the parameters chosen for comparison are the static temperature profile, the pitot pressure profile, and the distributions of mixing and heat release. The mixing parameter η_m is defined as the fraction of fuel mixed so that it could react completely. The heat release parameter η_{CR} is the difference in the heats of formation of the local and initial mixtures relative to the amount of heat available through conversion of all of the H_2 to water.



a) Static temperature profiles.



b) Pitot pressure profiles.



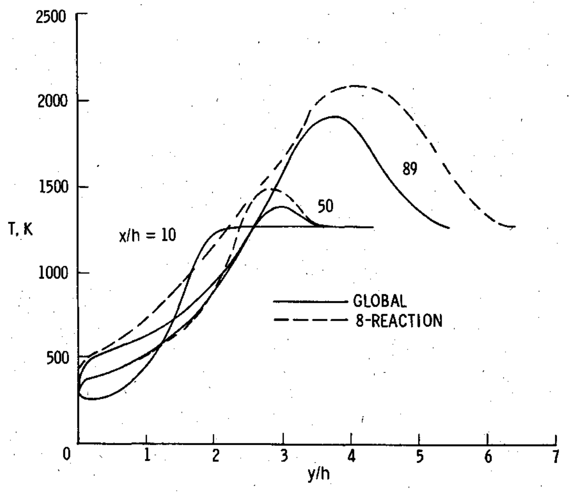
c) Mixing and heat release distributions.

Fig. 7 Comparison of global model with eight-reaction mechanism, case 1.

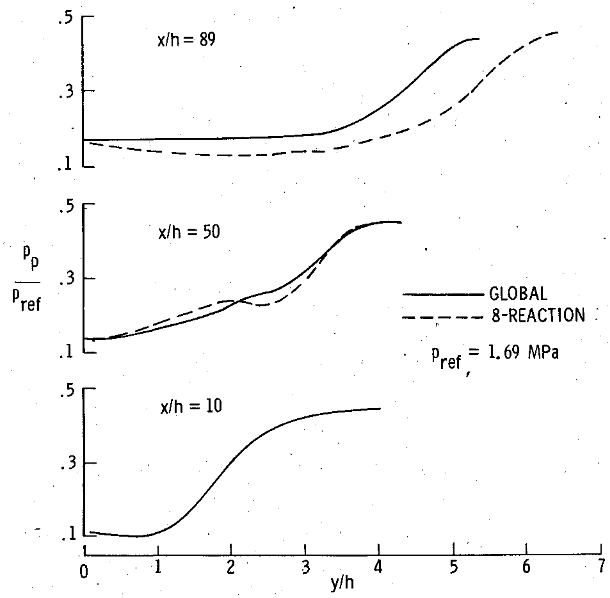
Test Case 1

Results obtained for the axisymmetric flowfield of case 1 are presented in Fig. 7. Radial profiles of the static temperature and pitot pressure are given at three axial locations. The pitot pressure is made dimensionless by a pressure $p_{ref} = 0.68$ MPa, which is the stagnation pressure of the mainstream air. The agreement between the profiles using the global model (solid lines) and the eight-reaction mechanism (broken lines) is considered to be quite good. For the mixing and heat release distributions in Fig. 7c the agreement is also acceptable.

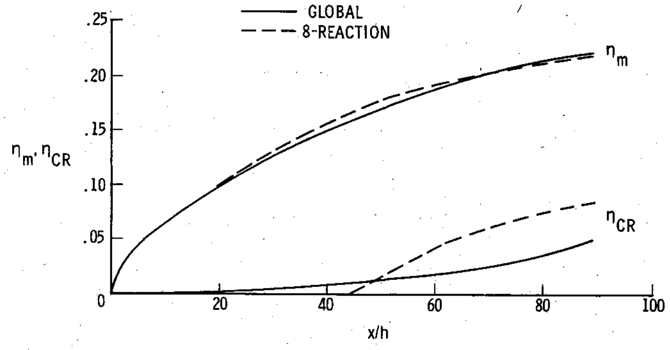
The implication of the good agreement illustrated by these comparisons is that the global model approximates the



a) Static temperature profiles.

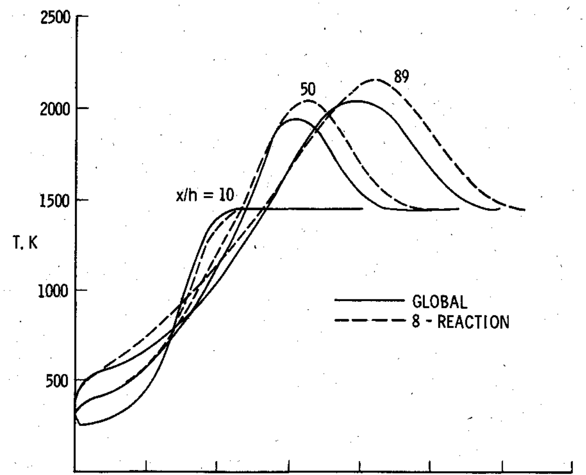


b) Pitot pressure profiles.

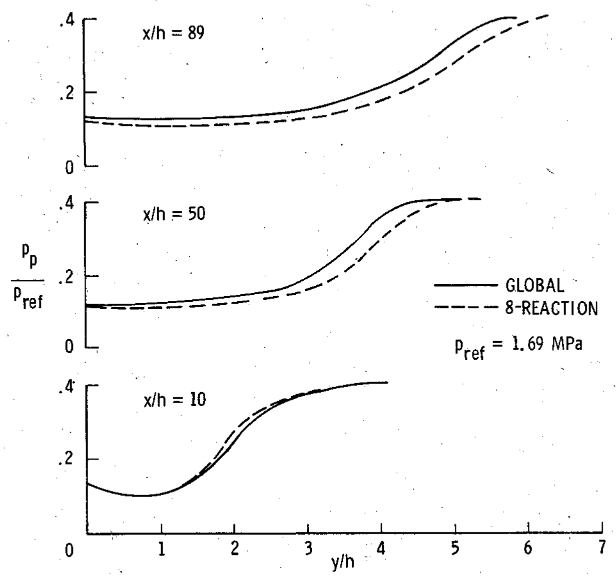


c) Mixing and heat release distributions.

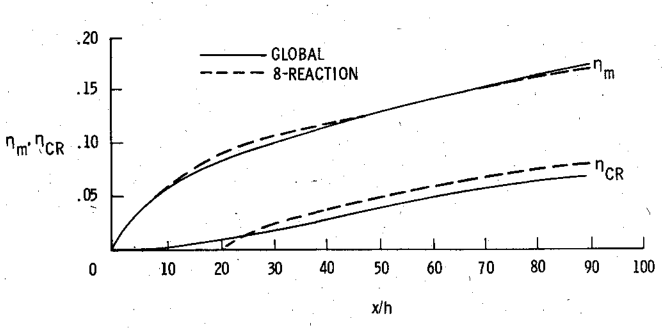
Fig. 8 Comparison of global model with eight-reaction mechanism, case 2A, $T_0 = 1270$ K.



a) Static temperature profiles.



b) Pitot pressure profiles.



c) Mixing and heat release distributions.

Fig. 9 Comparison of global model with eight-reaction mechanism, case 2B, $T_0 = 1450$ K.

chemistry of the flame without altering the diffusion process. Although the heat release of the global model is less than that for the eight-reaction mechanism, only about 18% of the hydrogen fuel has mixed to a reactable concentration at the $x/d_j = 27.9$ axial station. It is expected that as mixing proceeds, additional grid points within the mixing layer would have an equivalence ratio within the range of applicability of the global model. Thus, the global model would then be applied at more points, with a corresponding larger heat release and better agreement with the eight-reaction results.

Test Case 2

Results obtained for the two-dimensional flowfield of case 2 are presented in Figs. 8 and 9. For case 2A, in Fig. 8, the conditions are for a hydrogen jet at a temperature of 254 K and an air mainstream at a temperature of 1270 K. The profiles of static temperature and pitot pressure are plotted vs the transverse position in jet gap heights y/h. The reference pressure used to scale the pitot pressure is the mainstream air stagnation pressure with a value of 1.69 MPa. Agreement between the global model results (solid lines) and the eight-reaction results (broken lines) is acceptable in the near field, less than $x/h = 50$. However, at the $x/h = 89$ station, the profiles that result from the eight-reaction mechanism indicate much more reaction has occurred with more spreading of the fuel than for the global model results. A likely reason for this difference can be proposed by examination of the heat release distribution in Fig. 8c. Whereas the global model results indicate a gradual increase in the heat release with downstream distance, the eight-reaction results have no significant heat release until about $x/h = 45$. The implication is that the flow in the mixing layer does not ignite until this point. Downstream of the $x/h = 45$ ignition point, a sharp rise in the heat release occurs with corresponding temperature increase and more extensive spreading of the fuel. Note, however, that the mixing distributions in Fig. 8c indicate that there is no significant difference in the amount of fuel mixed to a reactable level. It should also be noted that the two-step global model was not intended to reproduce details of the ignition phase, but rather to replicate the overall combustion process. However, if the ignition delay is responsible, then raising the air temperature to a value near that of case 1, for which acceptable agreement was obtained, should result in better agreement.

To investigate this question, case 2B was computed, differing from case 2A only by having the temperature of the mainstream air raised to 1450 K. Calculations for this case, given in Fig. 9, show much better agreement between the global model and the eight-reaction mechanism. The agreement between the profiles of static temperature and pitot pressure is of the same quality as for the case 1, where the mainstream temperature was 1495 K. In Fig. 9c the heat release for the eight-reaction solution begins near $x/h = 20$. The global model heat release is lower, but agrees well with the trends of case 1. Since, as was discussed for case 1, only about 16% of the hydrogen has mixed to a reactable concentration, the implication that further mixing would increase the heat release for the global model and improve the agreement may also be suggested for this case.

Based on the comparisons of cases 2A and 2B it is concluded that the poor agreement for case 2A results from the inadequate representation of the long ignition delay time. However, good representation of the flow is possible with the global model for cases in which ignition does not dominate (cases 1 and 2B). Although only the relatively high-temperature cases showed good comparisons, the success of the global model for the stream tube calculation implies that the model will work at lower temperatures when ignition delays are not excessive. Future efforts will explore these issues more fully. One definite advantage to the global model is the reduction in complexity of the solution and the computer time to obtain a solution. A comparison of computer run times for these cases indicates a reduction in run times with the global model by a factor of four to five from that with the eight-reaction mechanism. These shorter run times can be an important factor in assessing the macroscopic behavior of a turbulent diffusion flow.

Conclusion

A two-step global model for the oxidation of hydrogen has been presented. The global model was established based on the criterion that it adequately reproduce the temperature history as given by a complete 28-reaction H_2-air mechanism. Arrhenius expressions for the rate constants were determined for a pressure of 1 atm, temperatures of 1000-2000 K, and mixtures 0.2-2.0 times stoichiometric.

The present global model was applied to the calculation of the turbulent combustion of a hydrogen jet in a supersonic airstream in both axisymmetric and two-dimensional geometries. Results of the calculations were compared with previous successful predictions of the flowfield data using an eight-reaction hydrogen-oxygen mechanism. Profiles of static temperature and pitot pressure were adequately duplicated with the global model for the axisymmetric flow case with a mainstream temperature of 1495 K. For the two-dimensional flow case with a mainstream temperature of 1270 K, the global model did not adequately reproduce the results with the eight-reaction mechanism. The apparent reason for this lack of agreement is a long ignition delay (about 50 jet heights). An increase in the mainstream temperature of 1450 K resulted in much better agreement. For both cases, the distribution of fuel mixed to a reactable concentration was well matched between the global model and the eight-reaction mechanism. However, the distribution of heat release with the global model lagged that with eight reactions but followed the proper trend.

Computational run times of the computer program with the global model were a factor of four to five times less than for the eight-reaction mechanism. Within the present range of applicability, the global model is considered to adequately predict the oxidation of hydrogen. Work is currently underway to extend the model to include pressure effects on the rate constant parameters, and to better define and expand the range of application.

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