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# SIMPLIFIED JET FUEL REACTION MECHANISM FOR LEAN BURN COMBUSTION APPLICATION

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## Abstract

Successful modeling of combustion and emissions in gas turbine engine combustors requires an adequate description of the reaction mechanism. For hydrocarbon oxidation, detailed mechanisms are only available for the simplest types of hydrocarbons such as methane, ethane, acetylene, and propane.[1,2] These detailed mechanisms contain a large number of chemical species participating simultaneously in many elementary kinetic steps. Current computational fluid dynamic (CFD) models must include fuel vaporization, fuel-air mixing, chemical reactions, and complicated boundary geometries.

To simulate these conditions a very sophisticated computer model is required, which requires large computer memory capacity and long run times. Therefore, gas turbine combustion modeling has frequently been simplified by using global reaction mechanisms, which can predict only the quantities of interest: heat release rates, flame temperature, and emissions.

Jet fuels are wide-boiling-range hydrocarbons with ranges extending through those of gasoline and kerosene. These fuels are chemically complex, often containing more than 300 components. Jet fuel typically can be characterized as containing 75 vol % paraffin compounds and 25 vol % aromatic compounds. A five-step Jet-A fuel mechanism which involves pyrolysis and subsequent oxidation of paraffin and aromatic compounds is presented here. This mechanism is verified by comparing with Jet-A fuel ignition delay time experimental data, and species concentrations obtained from flametube experiments. This five-step mechanism appears to be better than the current one- and two-step mechanisms.

## Introduction

Jet fuel oxidation involves a very large number of reaction species, thus a large number of differential equations are required to develop an acceptable kinetic mechanism. These differential equations are usually stiff and require special integration techniques. In addition, the specific rate constants of the elementary reactions either are not available in the literature, or are not necessarily well known and can be a potential source of error. The present kinetic mechanisms attempt to simplify the chemistry in order to predict quantities of interest, such as heat release rates, flame temperature, and concentration of important principal species such as unburned hydrocarbons, CO, and $CO_2$.

The simplified Jet-A chemical kinetics mechanism is based on the modified Arrhenius equation,

$$k = AT^n \exp(-E/RT) \tag{1}$$

where the rate k depends on the temperature T, temperature exponent n, an activation energy E, and a pre-exponential collision frequency factor A. The simplest Jet-A reaction mechanism is the one-step mechanism:

$$C_{13}H_{26} + 19.5O_2 \rightarrow 13CO_2 + 13H_2O \tag{2}$$

| A | n | E(Kcal/kg mol) |
|---|---|---|
| $7.5\times10^{10}$ | 0 | 41 000 |

The activation energy E value of 41 000 Kcal/kg mol has been reported by Freeman and Lefebvre[3] for kerosene fuel. The collision frequency factor A value of $7.5\times10^{10}$ has been determined by comparison with Jet-A fuel ignition delay time data. A slightly more complex mechanism is the two-step mechanism, which is very similar to what was proposed by Edelman and Fortune:[4]

$$C_{13}H_{26} + 13O_2 \rightarrow 13CO + 13H_2O \tag{3}$$

| A | n | E(Kcal/kg mol) |
|---|---|---|
| $3.37\times10^{11}$ | 0 | 41 000 |

$2CO + O_2 \rightarrow 2CO_2$

$$\frac{A}{3.48\times10^{11}} \quad \frac{n}{2} \quad \frac{E(Kcal/kg\ mol)}{20\ 140} \qquad (4)$$

The rate expression for the reaction (Eq. 4) is reported by Hautman and Dryer.[5] The collision frequency factor of $3.37\times10^{11}$ for reaction (Eq. 3) has been determined by comparison with Jet-A fuel ignition delay time data. However, neither of these mechanisms account for molecular hydrogen, and the predicted flame temperatures are higher than experimental results.

The proposed Jet-A fuel kinetic mechanism is represented by a five-step mechanism listed below. Initially the paraffin base hydrocarbon molecule is broken down into hydrocarbon fragments.[6] For simplicity, only one major hydrocarbon $C_2H_4$[7] will be tracked in this mechanism.

$2C_{13}H_{28} \rightarrow 13C_2H_4 + 2H_2$

$$\frac{A}{8.0\times10^{10}} \quad \frac{n}{0} \quad \frac{E(Kcal/kg\ mol)}{41\ 000} \qquad (5)$$

$C_{10}H_8 + 5O_2 \rightarrow 10CO_2 + 4H_2$

$$\frac{A}{2.4\times10^{11}} \quad \frac{n}{0} \quad \frac{E(Kcal/kg\ mol)}{41\ 000} \qquad (6)$$

$C_2H_4 + O_2 \rightarrow 2CO + 4H_2$

$$\frac{A}{2.2\times10^{9}} \quad \frac{n}{2} \quad \frac{E(Kcal/kg\ mol)}{28\ 600} \qquad (7)$$

$2CO + O_2 \rightarrow 2CO_2$

$$\frac{A}{3.48\times10^{11}} \quad \frac{n}{2} \quad \frac{E(Kcal/kg\ mol)}{20\ 140} \qquad (8)$$

$2H_2 + O_2 \rightarrow 2H_20$

$$\frac{A}{3.0\times10^{20}} \quad \frac{n}{-1} \quad \frac{(Kcal/kg\ mol)}{0} \qquad (9)$$

The rate expressions for the overall reactions (Eqs. (7) to (9)) are reported by Hautman and Dryer.[5] Reaction (5) is the overall paraffin compound pyrolysis step, and reaction (6) is the overall aromatic compound oxidation step. The value of the activation energy, E, of 41 000 Kcal/kg mol is reported by Freeman and Lefebvre for kerosene fuel. The values of collision frequency factor of $8.0\times10^{10}$ for reaction (5), and $2.4\times10^{11}$ for reaction (6) are determined by comparison with Jet-A fuel ignition delay time data. The full mechanism is based on the standard mechanism of Miller and Bowman[8] coupled with Eqs. (5) and (6). This mechanism involves 51 species and 242 reactions and requires significant computer resources, demonstrating the need for a reduced kinetic mechanism for engineering calculations.

Extensive measurements of species concentrations have been obtained from high pressure, high temperature flow reactor experiments. These data provided insight for the development of a new kinetic mechanism for jet-A fuel oxidation.

## Experimental Apparatus and Procedure

### Test Facility

The flametube combustor is mounted in the CE5B test facility, which is located in the Engine Research Building (Bldg. 5) at NASA Lewis Research Center. Tests were conducted with combustion inlet air pressure ranging from 10 to 15 atm (147 to 221 psia). A natural gas preheater is used to supply nonvitiated air at 755 to 866 K (900 to 1100 °F) inlet temperature. The temperature of the air is controlled by mixing the heated air with cold bypass air. Downstream of the combustor rig, quench water is sprayed into the gas stream to cool the exhaust to below 333 K (140 °F). Total pressure of the combustor, and airflow through the heat exchanger and bypass flow system are regulated by remotely controlled valves.

The fuel used for this work is specified by the ASTM Jet-A turbine fuel designation. This is a multicomponent kerosene-type fuel commonly used in gas turbine engines. Ambient temperature Jet-A, with a hydrocarbon ratio of 1.96, is supplied to the fuel injector. Flow rates are measured with a calibrated turbine flow meter and were varied from 0.1 to 4.0 GPM with a supply pressure of 650 psig.

### Test Rig

The high pressure and temperature test rig used in this experiment consists of an inlet section, fuel injection and vaporization section, flameholder, and combustion section. The combustor test rig is illustrated schematically in Fig. 1. The test section is square having an area of 58 $cm^2$ (9 $in.^2$). A square cross-sectional flametube was chosen based on the need to incorporate windows for nonintrusive diagnostic measurements. The premixed/prevaporization section, and the combustion section are 27 cm (10.5 in.) and 74 cm (29 in.) long, respectively. A ceramic refractory material is used as a liner in the combustion section. This insulating material enables the reactor to be characterized as a one-dimensional adiabatic plug flow reactor.

### Fuel Injector

Jet-A fuel is introduced into the airstream by means of a multiple-passage fuel injector shown in Fig. 2. The fuel injector was designed to provide good dispersion of fuel in the airstream by injecting equal quantities of fuel into each of the individual passages. The injector used in these tests has 16 square passages. Each passage was machined to form a converging/diverging flowpath. The 64-percent blockage helps to insure a uniform velocity profile over the entire flowfield. The pressure drop across the injector ranges between 3 and 6 percent of the inlet pressure.

### Flameholder

A 1.27 cm (0.50 in.) thick perforated plate flameholder, was made from Inconel 718, and is shown in Fig. 3. The plate, used to stabilize the flame, contains a staggered array of 36 holes, 0.64 cm (0.25 in.) in diameter, which results in a flow blockage of 80 percent. The holes have a smooth inlet radius on the upstream side of the plate, and a thermal barrier coating (ZrO) on the downstream side of the plate for extended thermal wear. The total pressure drop across the flameholder ranged from 5 to 12 percent of inlet air pressure.

### Combustion Section

The water-cooled combustion section has a square cross-sectional area of 58 $cm^2$ (9 $in.^2$), and is 74 cm (29 in.) long. A sketch of the cross section is shown in Fig. 4. For the inlet conditions listed above, adiabatic flame temperatures ranging from 1700 to 2089 K (2600 to 3300 °F) were measured in the combustor section. The flowpath is lined with a high temperature castable refractory material to minimize the heat loss. A high temperature, insulating, ceramic fiber paper is placed between the refractory material and the stainless steel water-cooled housing. The paper serves two purposes: (1) to reduce the heat loss and minimize cold-wall effects; and (2) to compensate for the difference in thermal expansion between the ceramic and the housing. The stainless steel housing is water-cooled through copper tubing coils wrapped and welded to its outer diameter.

### Instrumentation

The combustion gases are sampled with six water-cooled sampling probes located 10.2, 30.5, and 50.8 cm (4, 12, and 20 in.) downstream of the flameholder, as seen in Fig. 2. There are two probes at each axial location, with the top probes positioned 1.57 cm (0.62 in.) to the left of center (when looking downstream), and the bottom probes positioned the same distance to the right of center. The probes are 1.57 cm (0.62 in.) in diameter with five 1.02 mm (0.040 in.) I.D. sampling tubes manifolded together and terminating 1.51 cm (0.594 in.) apart along the probe length. Steam-traced stainless steel tubing, 6.4 mm (0.25 in.) O.D. and approximately 15.2 m (50 ft) in length, connect the gas sample probes to the gas analysis equipment. The steam tracing prevents the condensation of unburned hydrocarbons in the line. The probes are mounted on pneumatically operated cylinders interconnected with remotely operated solenoid valves, which allows two probe positions: in and out. The analysis of sample gas was performed by inserting only one probe into the combustion zone at a time, thus minimizing flow disturbances which could affect rig operation.

In addition to gas analysis, pressure and temperatures are measured along the test rig. At the exit of the inlet plenum, a rake containing five total pressure probes and a wall static tap are used to determine the air velocity profile. The inlet temperature is measured with two chromel/alumel thermocouples. Pressure and temperature are also measured upstream of the flameholder to determine the presence of upstream burning and the fuel injector pressure drop. The adiabatic flame temperature in the combustion section is measured using two platinum/rhodium thermocouples located 40.6 cm (16 in.) and 58.4 cm (23 in.) downstream of the flameholder. A pressure tap at the exit of the combustor is used to calculate the pressure drop across the flameholder and the combustion section.

## Validation of Mechanism

The experimental Jet-A oxidation results for this study were obtained using a flametube reactor. The flametube has a 3-in. by 3-in. test section, insulated by 2 in. of ceramic material. The experiments conducted were intended to be spatially homogeneous, so that radial transport effects may be neglected. Vaporization of injected liquid Jet-A fuel and mixing of the vaporized fuel with air was completed upstream of the flameholder.

Since inlet conditions control the degree of vaporization and mixing, they must be chosen carefully. In this study, an inlet temperature (Tin) of 1000 °F and inlet pressure (Pin) of 10 atm was chosen to assure total vaporization for equivalence ratios less than 0.6. The equivalence ratio was varied from 0.40 to 0.60. Recently, Lai[9] used a Phase Doppler Particle Analyzer to measure a mean droplet size of 40 $\mu$m for the fuel injector used in this study. Deur[10] then applied the KIVA-II code and predicted 100 percent vaporization before the fuel injector exit (Fig. 5) at Tin = 1025 °F, Pin = 142 psi, equivalence of 0.60, and SMD = 40 $\mu$m.

To study the fuel-air mixing effectiveness, a focused Schlieren technique has been used[11]. This provided a time-history of the flowfield at rates up to 10 000 frames/sec, using a high speed camera. Images from frames of the high speed film were digitized and color-enhanced to reveal regions of various density gradients (Fig. 6).

A method of extracting quantitative information from this type of image was devised. As shown in Fig. 6, if vertical lines are drawn at different axial stations in the flow, the degree of mixing as the flow proceeds downstream can be compared. Along each line, the mean and standard deviation of the image pixel intensities is found. A relatively low standard deviation is produced when there is little change in density gradients along the line. When a line cuts across a region of intense mixing, a higher standard deviation is found, as seen for example in lines D, E, and F. As the mixing is completed, line I crosses a more uniform flowfield and its standard deviation is lower. This method can be used to quantitatively compare degree of mixedness at various axial locations.

From these studies, the fuel-air mixture in the premixing section of the flametube was found to be prevaporized and premixed. The inlet fuel-air mixture velocity was constrained by requiring combustion to be stabilized, but still sufficient to result in turbulent conditions. The combustion wall was insulated, and the amount of Jet-A injected was less than 1 percent on a molar basis. Thus, the flametube reactor was characterized as one-dimensional plug flow reactor.

## Results

Four mechanisms were examined, they are: one-step, two-step, five-step, and full mechanisms. These four mechanisms were then integrated into the LSENS code[12] to perform case studies. Results from these case studies are shown in Figs. 7 to 10. Jet-A fuel ignition delay times (Fig. 7), flame temperatures (Fig. 8), and species concentrations (Figs. 9 and 10) for various equivalence ratios have been calculated. The calculated results from the full mechanism shows excellent agreement with experimental data as expected. The five-step mechanism produced reasonable agreement with experimental data, because $C_2H_4$ is the only intermediate hydrocarbon fragment assumed in this mechanism. All of the four mechanisms explained the increased carbon monoxide concentration with increase in equivalence ratio, but no quantitative comparison could be made.

## Summary

Flametube combustor experiments were conducted at an inlet pressure of 10 atm and inlet temperatures of 1000 to 1100 °F, and equivalence ratios ranging from 0.4 to 0.6. Calculated results from the proposed five-step mechanism indicated that our semiglobal simplified mechanism approach shows promise for use in combustor modeling codes. Work is continuing on improving the mechanism and testing it over a wider range of experimental conditions.

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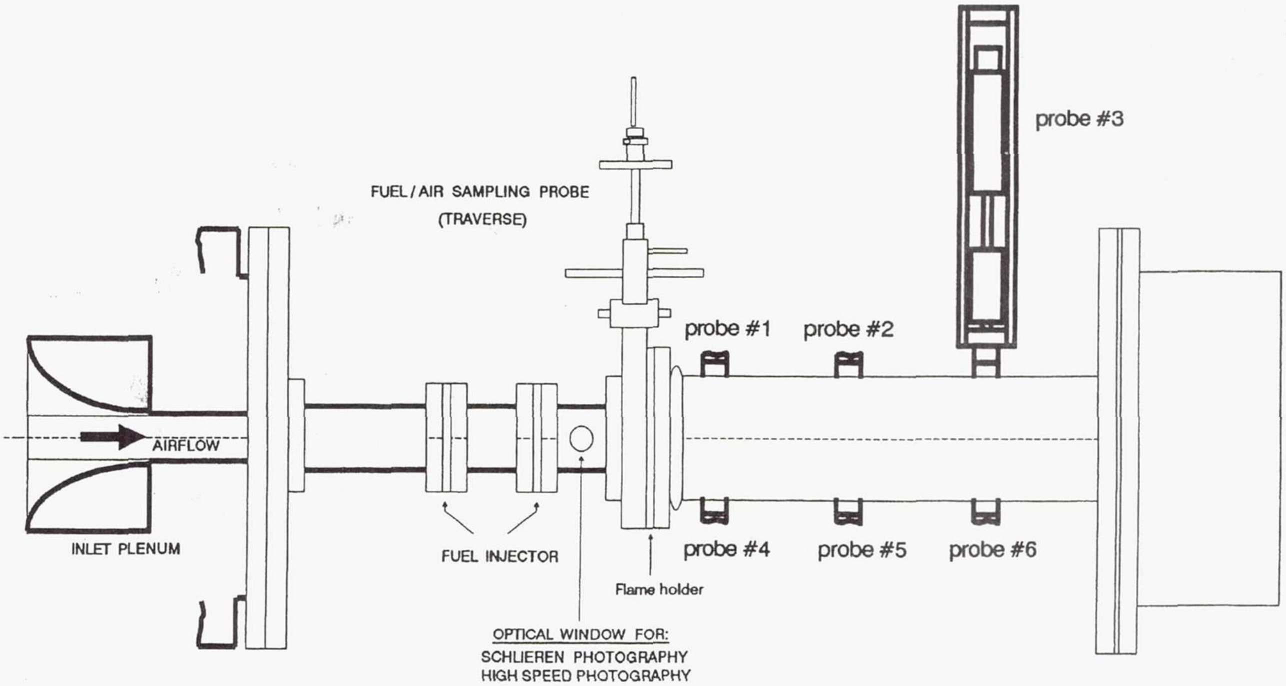


Figure 1.—High pressure and temperature flame tube combustor rig.

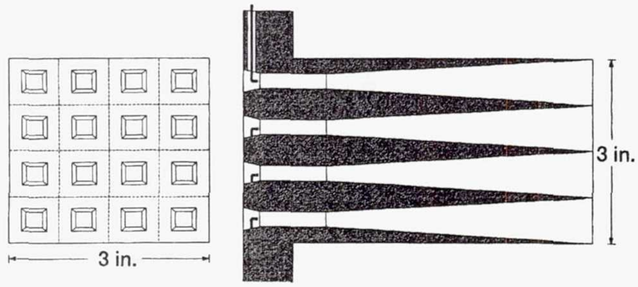


Figure 2.—Multiple tube fuel injector.

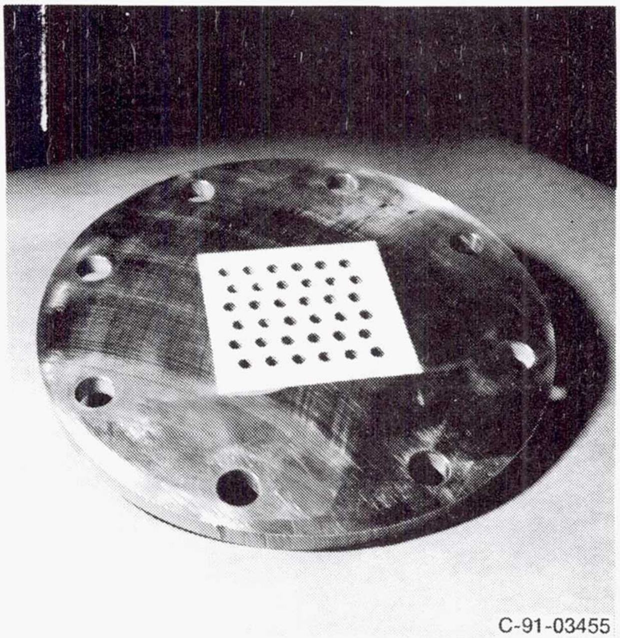


Figure 3.—Uncooled flame holder.

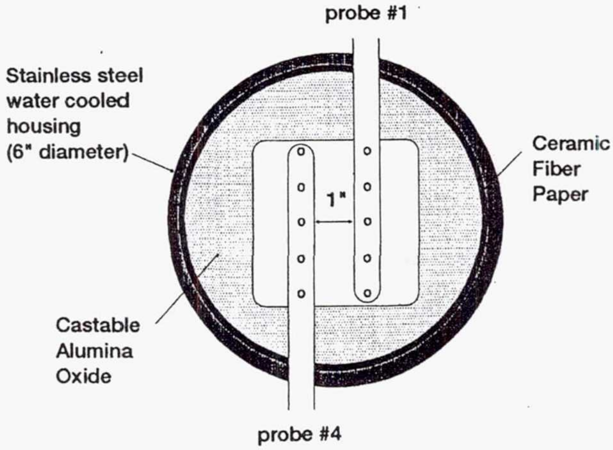


Figure 4.—Flame tube cross section and sampling probes.

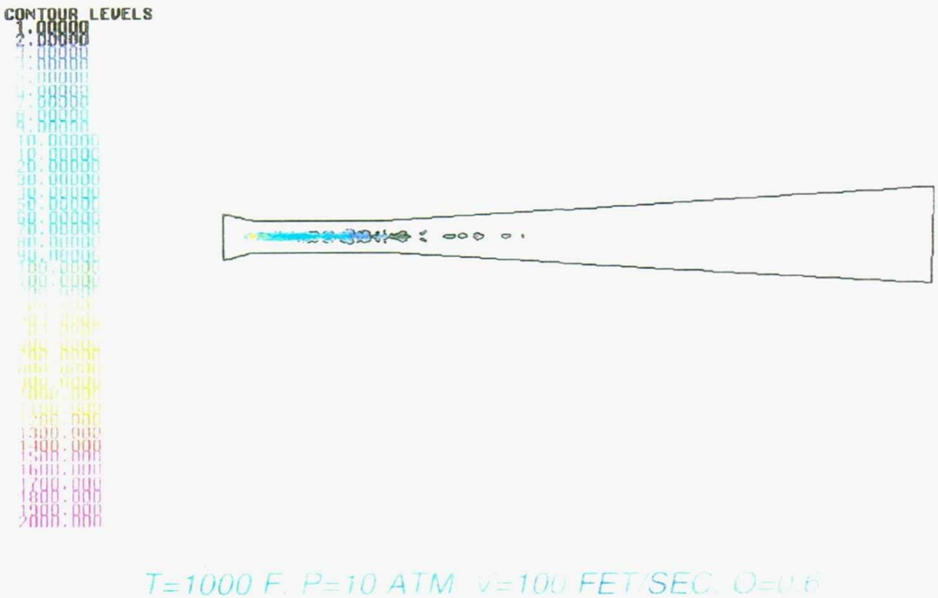


Figure 5.—Jet-A droplet population contours for venturi fuel injector.

| Line | Std. Dev. | Mean |
|---|---|---|
| A | 15.36 | 36.10 |
| B | 32.64 | 65.79 |
| C | 47.26 | 99.44 |
| D | 49.17 | 102.34 |
| E | 52.57 | 114.00 |
| F | 50.04 | 127.28 |
| G | 48.42 | 140.49 |
| H | 42.48 | 122.62 |
| I | 30.43 | 68.73 |

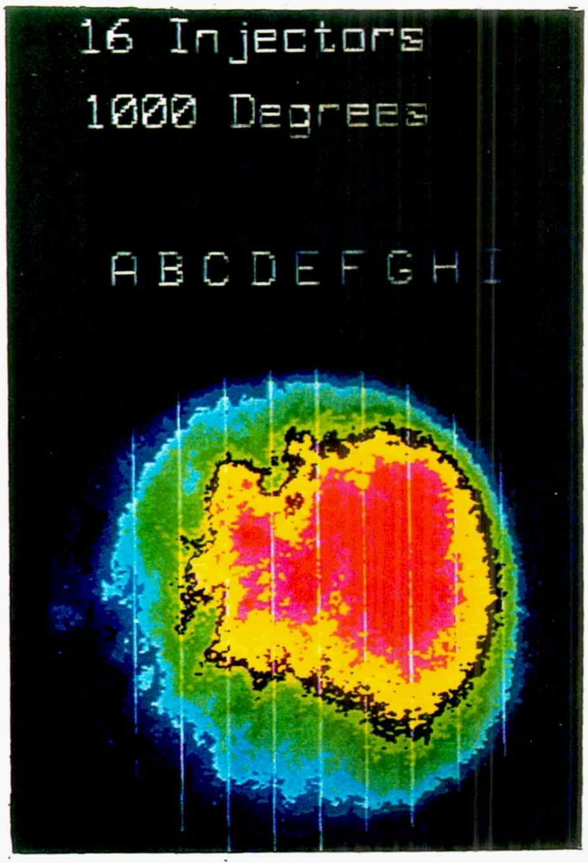


Figure 6.—Digitized flow field at premixed section.

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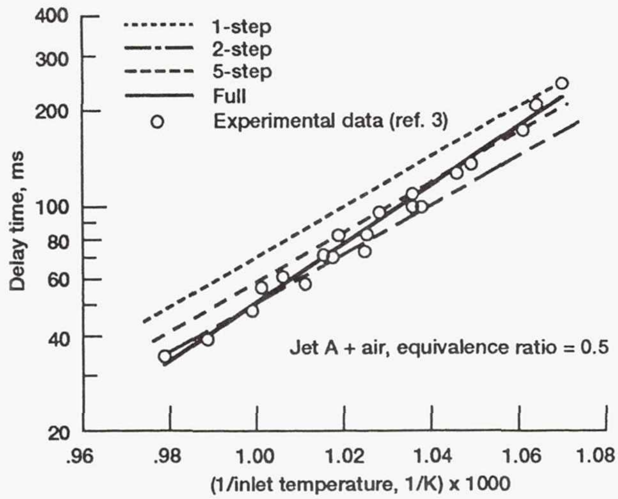



Figure 7.—Comparison of ignition delay times.

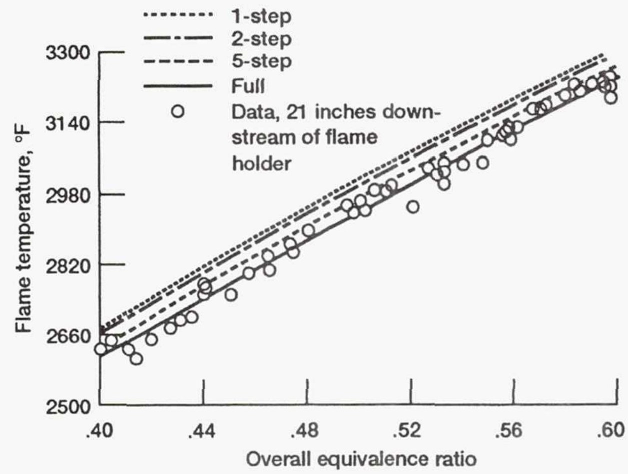
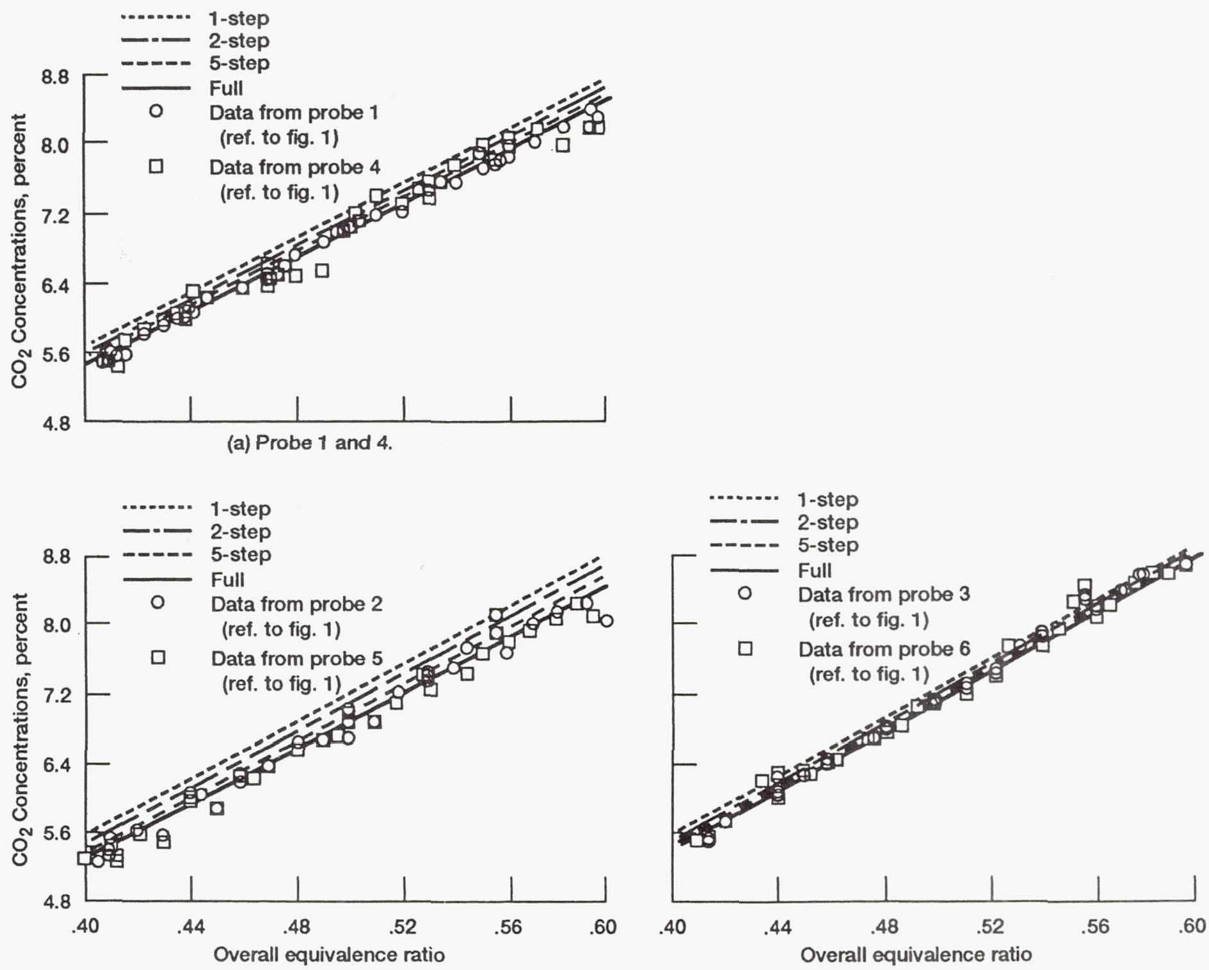



Figure 8.—Comparison of analytical & experimental flame temperatures.




(a) Probe 1 and 4.

(b) Probe 2 and 5.

(c) Probe 3 and 6.

Figure 9.—Comparison of analytical & experimental $CO_2$ concentrations.

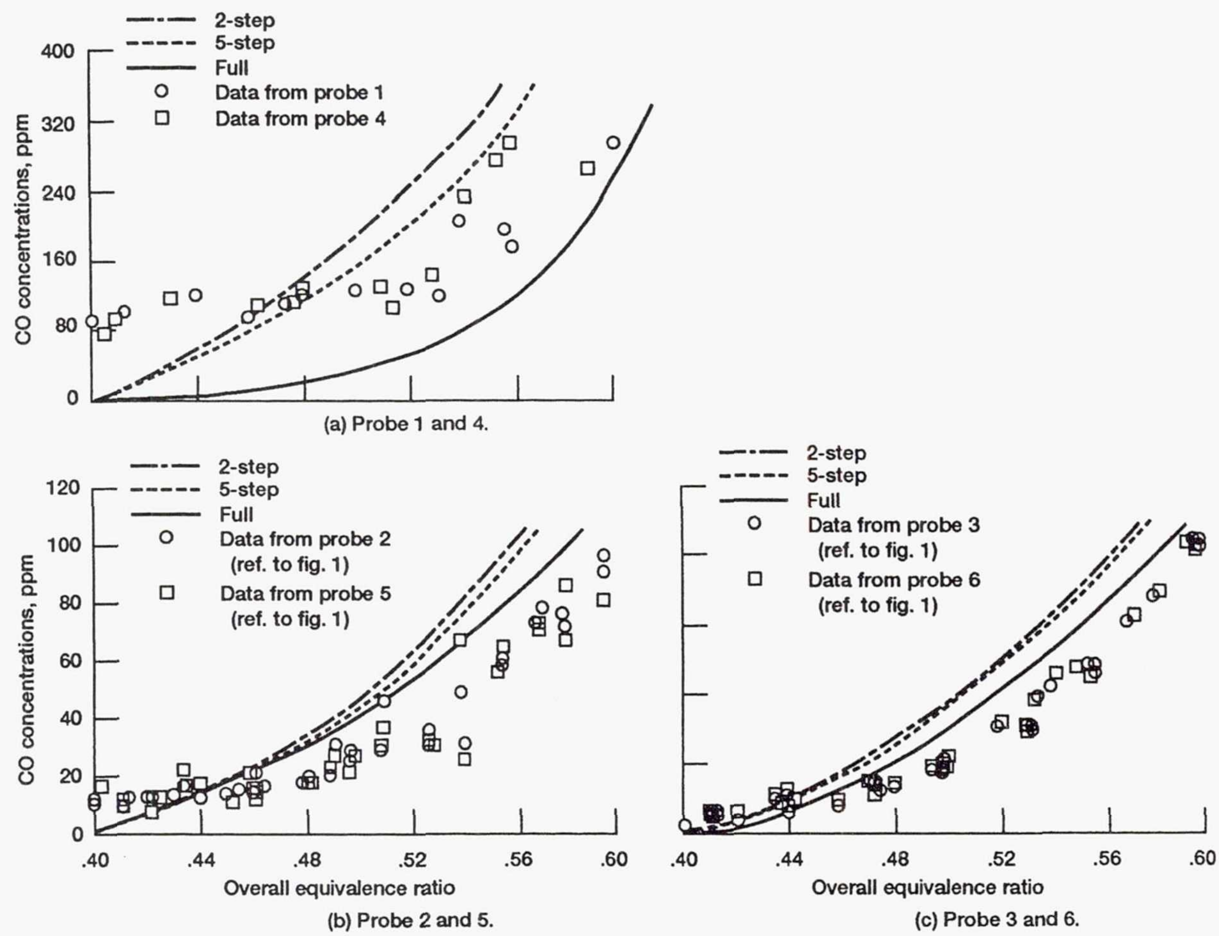



Figure 10.—Comparison of analytical & experimental CO concentrations.

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