Analytical and Experimental Investigation of an Ammonia/Air Opposed Reacting Jet

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Abstract—The point-by-point properties of an ammonia/air opposed-reacting-jet flowfield are described by solving the governing partial differential elliptic equations. Analytical descriptions of the reacting flowfield are compared to experimentally measured profiles of temperature and composition. Calculated distributions of stream function, temperature and fuel mole fraction are also presented.

NOTATION

| Symbol | Description | Subscript | Notes |
|--------|-------------|-----------|-------|
| \( A \) | pre-exponential factor in reaction rate expression | | |
| \( c_v \) | specific heat, Btu/lbm-\(^{\circ}\)R | | |
| \( D \) | combustor diameter, in. | | |
| \( \mathcal{D} \) | mass diffusivity | | |
| \( E \) | activation energy, Btu/lbm-mole | | |
| \( f \) | reaction order with respect to ammonia | | |
| \( H_C \) | heat of combustion, Btu/lbm | | |
| \( h \) | stagnation enthalpy, Btu/lbm | | |
| \( K \) | constant in effective viscosity expression | | |
| \( k \) | thermal conductivity, Btu/hr-ft-\(^{\circ}\)F | | |
| \( L \) | length of flow field, ft. | | |
| \( m \) | mass fraction | | |
| \( m \) | mass flow rate, lbm/sec | | |
| \( n \) | overall reaction order | | |
| \( R_{\text{et}} \) | reaction rate, lbm\(s^-1\)/sec | | |
| \( \mathcal{R} \) | universal gas constant, 1545 ft-lbf/lbm-mole-\(^{\circ}\)R | | |
| \( r \) | radius, in. | | |
| \( T \) | temperature, °F or °R | | |
| \( v \) | velocity, fps | | |
| \( \Gamma \) | exchange coefficient | | |
| \( \mu \) | viscosity | | |
| \( \rho \) | density, lbm/ft\(^3\) | | |
| \( \sigma_{\text{et}} \) | Schmidt Number | | |
| \( \sigma_h \) | Prandtl Number | | |
| \( \sigma \) | stress tensor | | |
| \( \Phi \) | equivalence ratio | | |
| \( \phi \) | dependent variable | | |

INTRODUCTION

An opposed-reacting-jet (ORJ) is shown in Figure I. The flame is stabilized by a jet directly opposing the premixed combustible main flow. The jet stream can be air, a fuel/air mixture or an inert gas. The flame will blow out when the jet is shut-off. Because the flame is stabilized by the jet, the opposed-reacting-jet is classified as a flameholder.

In this investigation, the governing partial differential equations are solved for an ammonia/air opposed-reacting-jet. Solutions are compared to experimental measurements. The objective is to demonstrate that the governing equations can be solved for a reacting, turbulent flow with recirculation while obtaining satisfactory correlation with experiment. A theoretical prediction of
A flame requires a reactive composition and an igniting condition. To occur, a flame needs a continuing feed of reactant mixture and a sufficient reflux of energy and/or active species.

A steady-state flame represents a balance between chemical reaction, fluid mechanics, mass diffusion, and heat conduction. The balance cannot be sustained indefinitely as the mass flow rate of reactants is increased. A critical flow rate (or velocity) will be reached above which insufficient energy will be recirculated upstream to sustain the flame, and the flame will consequently blow out. The critical velocity is on the order of the flame propagation rate. Velocities higher than the flame propagation rate occur often in actual combustion systems (e.g., the ramjet and the after-burner of a gas-turbine engine) and special devices called flameholders must be used to stabilize the flame.

In Figure 2, streamlines ($\psi = \text{constant}$) are plotted for a selection of flameholder configurations. The flameholder acts to decelerate the stream locally and provide a zone of recirculation. The recirculation zone is characterized by a reverse flow. Partially or completely reacted species are recirculated upstream to the region of decelerated flow. The zone of recirculation provides the necessary energy to sustain the flame.

The flameholders shown in Figure 2 are referred to as “physical” flameholders. Another class of flameholders are called “aerodynamic” flameholders. The opposed-reacting-jet shown in Figure 1 is an example of the aerodynamic type. The flame is stabilized near the stagnation region of the main and jet streams. The zone of recirculation...

FIG. 1. Aerodynamic flameholder, the opposed reacting jet.

FIG. 2. Physical flameholders.
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is located along the edge of the jet. The stream exiting the jet tube entrains and recirculates both partially and completely reacted species back to the region of stagnation.†

Although a flameholder will stabilize a flame at a velocity in excess of the flame propagation rate, the flame will eventually blow out as the approach stream velocity is increased. The velocity at which the flame blows out is called the blowout velocity. The blowout velocity depends on the equivalence ratio‡ of the approach stream. This dependency is illustrated by the blowout map shown in Figure 3 for an ammonia/air ORJ with a stoichiometric jet.

As shown in Figure 4, the blowout velocity depends on the jet composition as well as the main stream composition. The influence of the jet composition distinguishes the ORJ from a physical flameholder. Only one blowout map can be generated for a physical flameholder whereas a series of blowout maps can be generated for an ORJ by changing the jet composition.

The ORJ, first introduced in the open literature by Schaffer and Cambel (1955), was conceived as a potential flameholder in an afterburner of a gas turbine engine. The conventional physical flameholder produces drag losses when the afterburner is not in use. To negate these aerodynamic losses, Schaffer and Cambel proposed that the ORJ flameholder might be employed. Introduced at an angle from the wall of the afterburner, the jets could be shut off when the afterburner is not in use, leaving a streamlined wall.¶

The investigations of the ORJ have been primarily experimental. In the late 1950’s the Aircraft Division of General Electric sponsored a three-year investigation at Northwestern University. During the same period, the Air Force sponsored a program at Stanford Research Institute. Partly because interest swung to high-temperature gas dynamics in the early 1960’s and partly because the potential of the ORJ as a flameholder in afterburners was not realized, ORJ studies were

† The ORJ did not prove to be practical for use in afterburners because the flameholding capacity was found to decrease significantly as the angle of the jet to the direction of flow increased a few degrees (Duclos et al. 1957).

‡ The equivalence ratio, Φ, is defined as the actual fuel/air ratio divided by the stoichiometric fuel/air ratio

Φ = \( \frac{m_f}{m_a} / \left( \frac{m_f}{m_a} \right)_{stoch} \)

A stoichiometric mixture has an equivalence ratio of unity. Fuel-rich mixtures have equivalence ratios greater than unity and fuel-lean mixtures have ratios less than unity but greater than zero.

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FIG. 4. Blowout map: effect of jet composition (Schaffer, 1957).
curtailed with the exception of a program at Tulane University funded by the U.S. Army in the late 1960's (O'Loughlin, 1968).

STATE OF THE ART

Theoretical analyses of reacting flows with recirculation have in general been limited to modeling because of the inherent difficulties in solving the governing equations. For example, the stabilization of the bluff body (Longwell et al. 1953) and opposed-jet (Bellamy, 1966) flameholders has been likened to that of a stirred reactor. Similarly, gas turbine combustion has been modeled as a number of stirred reactors in series (Hammond and Mellor, 1970).

More effective characterization of pollutant formation in continuous combustion devices with recirculation requires the prediction of the point-by-point properties. Modeling is effective in predicting the performance of combustion systems, but is not wholly adequate in describing the detail of the flow field. The point-by-point properties of a reacting flow can be described only by a solution of the governing partial differential equations. In the case of flows with recirculation, similar to those of the opposed-jet and gas-turbine combustors, the equations are "elliptic."

Solution of the governing equations requires development of a numerical technique. Elliptic partial differential equations have been solved numerically for low-velocity flows, but difficulties are encountered with stability for Reynolds numbers above 400. In practice, the Reynolds number is often much higher. For the opposed-reacting-jet, Reynolds numbers based on the diameter of the combustor in excess of 10^4 are typical.

By giving special consideration to the formulation of the finite-difference equations, Runchal and Wolfshtein (1966) were successful in obtaining solutions to the elliptical equations that were stable for all Reynolds numbers. Instead of using the central difference formulation, they employed upwind difference formulation, a procedure suggested by Spalding (1966). The work of Runchal and Wolfshtein has led to the numerical technique adopted in the present study (Gosman et al. 1969).

ANALYTICAL INVESTIGATION

Conditions investigated

Two parameters are invariant in this investigation: the equivalence ratio of the jet, and the equivalence ratio of the main stream.

The fuel selected for this study was ammonia in part because the ammonia/air reaction can be adequately represented by a single-step or global reaction rate. The use of ammonia as the fuel is in contrast to previous work on the ORJ where hydrocarbons have been used exclusively, particularly propane. Intermediates such as aldehydes and carbon monoxide play an important role in hydrocarbon/air reactions, and at least two or three reactions and many species must be considered. As a result, hydrocarbon/air reactions are not as simple to describe as the ammonia/air reaction.

The ammonia/air reaction is assumed to follow the stoichiometry

\[
\text{(1) } 4\text{NH}_3 + 3\left[2\text{O}_2 + (3.77)\text{N}_2\right] \rightarrow 6\text{H}_2\text{O} + 13.31\text{N}_2
\]

The blowout map obtained experimentally for the ammonia/air opposed reacting jet is given in Figure 3. Numerical solutions to the governing equations were obtained for three cases:

Case 1: Cold flow† for the blowout conditions represented by point A
Case 2: Cold flow for the conditions represented by point B
Case 3: Hot flow for the conditions represented by point B

Governing equations

The partial differential equations that must be considered in solving the opposed-jet flowfield in the absence of combustion (cold flow) are the conservation of mass and the conservation of momentum. When the flowfield is nonisothermal due to chemical reaction, the conservation of energy must be added. Because individual species are created as well as destroyed through chemical reaction, conservation equations for each species must likewise be considered.

Using tensor form, the governing conservation equations may be written in the absence of body forces as:

\[
\text{Conservation of mass } \quad \text{div } \rho v = 0 \quad (2a)
\]

\[
\text{Conservation of momentum } \quad -\text{div } \rho vv - \text{grad } p - \text{div } \tau = 0 \quad (2b)
\]

† Cold flow: Nonreacting, isothermal flow. Hot flow: Reacting flow.
Conservation of energy
\[
\text{div} \{ \rho \mathbf{u} h - \Gamma_a c_n \text{grad} T \} \\
- h_{tu} \Gamma_{tu} \text{grad} m_{tu} - \sum_{i=1}^{3} u_i \tau_i = 0 \quad (2c)
\]

Fuel mass species conservation
\[
\text{div} \left( \rho \nu m_{tu} - \Gamma_{tu} \text{grad} m_{tu} \right) - R_{tu} = 0 \quad (2d)
\]

Normally a mass species conservation equation would be required for each of the species considered. Species-conservation equations for species other than the fuel species need not be solved here because the products are lumped together and considered as a whole, and the equivalence ratio is uniform throughout the flow field.

When the products are considered as a whole, the reaction assumes the following form:
\[
4 \text{NH}_3 + 3 \text{O}_2 \rightarrow \text{"product"} \quad (3)
\]

The oxidizer mass fraction need not be considered separately as a dependent variable as it is related algebraically to the fuel mass fraction through the equivalence ratio (based upon oxidizer mass fraction), \( \Phi \)
\[
m_{ox} = \frac{m_{tu}}{\Phi(m_{tu}/m_{ox})_{stoich}} \quad (4)
\]
The equivalence ratio is uniform and equal to unity throughout the flow field. Finally, the product mass fraction is known from
\[
m_{prim} = 1 - m_{tu} - m_{ox} \quad (5)
\]

The normal procedure is to transform or combine various of the governing equations into more convenient forms. The momentum equations in the radial and axial directions are combined to eliminate the pressure terms and most of the velocity terms. Performing this operation creates a new variable, vorticity \( \omega \). In cylindrical geometry, it is convenient to replace \( \omega \) as the dependent variable by \( \omega/r \). A second manipulation normally undertaken is to introduce the stream function, \( \psi \), defined by
\[
\rho \mathbf{u}_z = -\frac{1}{r} \frac{\partial \psi}{\partial r} ; \quad \rho \mathbf{u}_r = -\frac{1}{r} \frac{\partial \psi}{\partial z} \quad (6)
\]

into the continuity equation and into the other governing equations wherever velocity appears. The preceding manipulations result in four equations and four dependent variables:

- stream function, \( \psi \)
- vorticity variable, \( \omega/r \)
- stagnation enthalpy, \( \tilde{h} \)
- fuel mass fraction, \( m_{tu} \)

The equations for each of these dependent variables have a similar structure. For axi-symmetric flow, the general form is represented by:
\[
a_\phi \left( \frac{\partial}{\partial r} \left( \phi \frac{\partial \psi}{\partial r} \right) - \frac{\partial}{\partial z} \left( \phi \frac{\partial \psi}{\partial z} \right) \right) - \frac{\partial}{\partial z} \left( \phi^2 \frac{\partial \psi}{\partial z} \right) - \frac{\partial}{\partial r} \left( b_\phi \frac{\partial \psi}{\partial r} \right) + d_\phi = 0 \quad (7)
\]
The functions \( a_\phi, b_\phi, c_\phi, \) and \( d_\phi \) are given in Table I for each of the dependent variables, \( \phi \), considered.

**TABLE I**

| \( \phi \) | \( a_\phi \) | \( b_\phi \) | \( c_\phi \) | \( d_\phi \) |
|---|---|---|---|---|
| \( \psi \) | 0 | \( \frac{1}{\rho r} \) | 1 | \( -\omega \) |
| \( \omega/r \) | \( r^2 \) | \( r^2 \) | \( \mu_{ettr} \) | \( -r^2 \left( \frac{\partial}{\partial z} \left( \frac{u_r^2 + \omega_r^2}{2} \right) \frac{\partial \rho}{\partial r} \right) \)
+ \( \frac{\partial}{\partial r} \left( \frac{(1 - 1/\alpha_n) \frac{\partial u_r^2}{\partial r}}{\sigma_n} \frac{\partial m_{tu}}{\partial z} \right) \) \| \( \frac{\partial}{\partial z} \left( \mu_{ettr} \left( \frac{1 - 1/\alpha_n}{\sigma_n} \frac{\partial u_r^2}{\partial r} + \frac{1}{\sigma_n} \frac{\partial m_{tu}}{\partial r} \right) \right) \)
| \( \tilde{h} \) | 1 | \( r \Gamma_{tu} \) | \( \mu_{ettr} \) | 1 | \( -\frac{\partial}{\partial z} \mu_{ettr} \left[ \frac{1}{\sigma_n} \frac{\partial u_r^2}{\partial r} + \frac{1}{\sigma_n} \frac{\partial m_{tu}}{\partial r} \right] \)
+ \( \sigma_n \frac{\partial m_{tu}}{\partial z} \) \| \( \frac{\partial}{\partial r} \left( \mu_{ettr} \left( \frac{1 - 1/\alpha_n}{\sigma_n} \frac{\partial u_r^2}{\partial r} + \frac{1}{\sigma_n} \frac{\partial m_{tu}}{\partial r} \right) \right) \)
| \( m_{tu} \) | 1 | \( r \Gamma_{tu} \) | \( \mu_{ettr} \) | 1 | \( -\frac{\partial}{\partial r} \mu_{ettr} \left( \frac{1 - 1/\alpha_n}{\sigma_n} \frac{\partial u_r^2}{\partial r} + \frac{1}{\sigma_n} \frac{\partial m_{tu}}{\partial r} \right) \)
| \( \mu_{ettr} \) | 1 | \( r \Gamma_{tu} \) | \( \mu_{ettr} \) | 1 | \( -\frac{\partial}{\partial r} \mu_{ettr} \left( \frac{1 - 1/\alpha_n}{\sigma_n} \frac{\partial u_r^2}{\partial r} + \frac{1}{\sigma_n} \frac{\partial m_{tu}}{\partial r} \right) \)
Finite difference equations

The derivation of the finite difference equation from the governing partial differential equations is described by Gosman et al. (1969) and summarized for the particular case of the ORJ by Samuelsen (1970).

Before a solution to the problem may be obtained, certain accessory data—density, effective viscosity, chemical kinetics and specific heat—must be specified. The problem of turbulence is handled by adopting the method of time-averaged properties (Bird et al. 1960). The equations written for laminar flow are taken to apply, but the transport properties are replaced by the so-called “effective” transport properties. An example is the effective viscosity.

Effective viscosity: \( \mu_{\text{eff}} \)

The effective viscosity has been the focus of much attention in recent years. Most of the emphasis has been directed toward models for parabolic flows. Effort has recently been directed toward modeling the effective viscosity for elliptic flows. For the current study, the following model was adopted

\[
\mu_{\text{eff}} = K D^{2/3} L^{-1/3} \rho^{2/3} (\bar{v}_{\text{in}})^{1/3}
\]

Equation 8 is derived by dimensional analysis after specifying that the effective viscosity is influenced by \( \rho, L, D \) and \( (\bar{v}_{\text{in}}) \) in the following manner (Odlozinski, 1968):

- \( \rho \): \( \mu_{\text{eff}} \) increases with local density
- \( L \): \( \mu_{\text{eff}} \) diminishes with an increase in the length of the flow region
- \( D \): \( \mu_{\text{eff}} \) increases with the diameter of the flow region
- \( \bar{v}_{\text{in}} \): \( \mu_{\text{eff}} \) increases with the incoming rate of kinetic energy

Equation 8 has been used to predict reacting flows with recirculation by Pun and Spalding (1967) and Odlozinski (1968).

The advantages of using the simple model are threefold:

1. The simple model is economical to use; additional partial differential equations are not required, saving iteration time.
2. A design engineer or research engineer is often willing to sacrifice accuracy for the sake of economy, particularly as a first approximation to the solution of the problem.
3. The simple model provides a convenient reference against which more sophisticated models can be assessed.

Effective Prandtl and Schmidt numbers

The effective Prandtl and Schmidt numbers

\[
\sigma_{h, \text{eff}} = \frac{\Gamma_{h, \text{eff}}}{\mu_{\text{eff}}}, \quad \sigma_{\text{Tu, eff}} = \frac{\Gamma_{\text{Tu, eff}}}{\mu_{\text{eff}}}
\]

are taken to be unity, a convention adopted in prior studies involving turbulent elliptic flows (Odlozinski, 1968; Pun and Spalding, 1967).

For gases in both laminar and turbulent flows, the effective Prandtl and Schmidt numbers are typically in the vicinity of 0.7 (Shapiro, 1954). Using a value of unity in lieu of 0.7 has the advantage of simplifying the governing partial differential equation for enthalpy.

Chemical kinetics: \( d \)

The source term, \( d \), for the fuel mass fraction is functionally dependent on the chemical reaction rate, \( R_{\text{Tu}} \) (ref. Table 1). Adopting common convention, an Arrhenius form gives

\[
R_{\text{Tu}} = A_{\text{Tu}} \rho_{\text{in}}^{m_{\text{Tu}}} \rho^{n} \exp \left( -\frac{E}{RT} \right) \left[ \frac{\text{lbm}_{\text{Tu}}}{\text{ft}^{3} \text{sec}} \right]
\]

where \( A, n, f, \) and \( E \) are empirically determined constants. The rate data for the ammonia/air reaction studied here were taken from a well-stirred reactor study by Pratt and Starkman (1969). For the following stoichiometry

\[
4\text{NH}_{3} + 3\text{O}_{2} \rightarrow 6\text{H}_{2}\text{O} + 2\text{N}_{2}
\]

the constants in equation 10 assume the values:

\[
A = 2.5 \times 10^{10}, \quad f = 0.75, \quad n = 1.95, \quad E = 6.26 \times 10^{4} \text{ Btu/lbm-mole}
\]

The reaction rate presented in the Arrhenius form depends on the local time-mean gas properties. In reality, the local gas properties (e.g. velocity, pressure, etc.) fluctuate due to the eddy motion of turbulent flow. The reaction rate is not simply dependent on the time-smoothed properties, but may be strongly affected and, in fact, limited by the break-up of large eddies into small ones (Spalding, 1971). It might be expected then to find that the Arrhenius equation and well-stirred reactor data
given above do not give results quantitatively consistent with experimental findings. As a result, the data of Pratt and Strakman were used as first guesses. The constants $A$ and $E$ were then refined by comparing the numerical prediction to the experimental results.

**Heat of combustion: HC**

The heat of combustion for the ammonia/air reaction is evaluated from an enthalpy balance between the reactants and products and assuming that they combine in the proportion given by equation 1. For a temperature of 538 °R and using the data provided by the JANAF Tables (1960) the heat of combustion obtained is

$$HC = -8050 \text{ Btu/lbm}_{\text{NH}_3}$$

The choice of the reaction temperature is not important. The heat of combustion is nearly independent of temperature. For example, at 3500 °R, the enthalpy of reaction is $HC = -8091 \text{ Btu/lbm}_{\text{NH}_3}^\circ$.

**Specific heat**

Assuming that the specific heat of all the species is constant and equal, the following simplified temperature-rise relation is obtained

$$T = \frac{h - m_{\text{fl}}HC}{c_{p_{\text{mix}}}} \tag{12}$$

The fuel mass fraction, $m_{\text{fl}}$ and $h$, the enthalpy of the mixture are dependent variables and the heat of combustion is specified above. Only the specific heat, $c_{p_{\text{mix}}}$, needs yet to be specified.

The value adopted for the uniform and constant specific heat for all the species was

$$c_{p_{\text{mix}}} = 0.395 \text{ Btu/lbm}^\circ \text{R} \tag{13}$$

This value was calculated from equation 12 for the case of complete combustion ($m_{\text{fl}} = 0.0$) and the adiabatic flame temperature for the ammonia/air reaction of 3460 °R. The value for specific heat given by equation 13 compares favorably to that calculated (0.392) using the thermochemical data of the JANAF Tables (1960) at 3460 °R for the actual product species [6H$_2$O + 13.31N$_2$]. For the reactant species [4NH$_3$ + 3O$_2$ + 11.31N$_2$] at the inlet temperature of 538 °R the specific heat given by Equation 13 is thirty percent higher than the actual (0.290).

**COMPUTATIONAL PROCEDURE AND RESULTS**

Solutions were obtained for the two inlet main stream velocities. These two conditions are designated as points $A$ and $B$ in Figure 3. Point $A$ is located at the peak of the blowout curve, point $B$ is located at an approach velocity about 80 percent of the peak velocity.

**Grid**

To minimize computational time and still effectively cover the area of steep gradients, a nonuniform grid was employed. A schematic of the grid is given in Figure 5. (The grid is expanded by a factor of two in the $J$-direction to accentuate the detail near the centerline.) The grid is non-uniform in both directions. There are 15 nodes in the $J$-direction and 33 nodes in the $I$-direction. The jet exit plane is located at $J = 10$. The inner diameter of the jet exit is located at $J = 3$ and the outer diameter at $J = 6$.

**Reaction rate**

The constants $A$ and $E$ in the chemical rate expression (equation 10) were refined by comparing the numerical predictions to the experimental results. This procedure, described in the next section, resulted in the following values for $A$ and $E$:

$$A = 22.0 \times 10^{10}$$

$$E = 6.00 \times 10^{10} \text{ Btu/lbm-mole}$$

$$R_{\text{fl}} = 22.0 \times 10^{10} m_{\text{fl}}^{0.75} m_{\text{N}}^{1.3} p^{1.05} \times \exp\left(-6.00 \times 10^{4}/\tilde{R}T\right) \tag{14}$$

**Stream function distribution**

The stream function distributions for the three cases considered are presented in Figure 6. In

**FIG. 5. Grid.**
Figure 6a, the stagnation point is located 1$\frac{3}{4}$ inches upstream of the jet exit for Case 1 (cold flow at the blowout velocity). For Case 2, the stagnation point is located further upstream ($2\frac{3}{4}$ inches) than in the previous case. The difference in the location of the stagnation point is attributed to the lower approach velocity in Case 2.

The stream function distribution for the case of hot flow at point B is given in Figure 6c. The location of the stagnation point has moved upstream from the jet exit. The difference in the location of the stagnation point in the case of the reacting flow is attributed to the higher jet velocity. Although the jet mass flow rate is identical for both the hot and cold flow cases, the heating of the jet in the presence of combustion produces a jet velocity of 715 fps compared to a jet velocity of 294 fps in the case of cold flow.

**Temperature and composition distributions**

Temperature and fuel mole fraction distributions are plotted in Figure 7 for Case 3. A region of highly reacted species (fuel mole fraction = 0.004) and uniform temperature (3500 °R) is located upstream of the stagnation point. The nose of the flame front, situated 3$\frac{3}{4}$ inches upstream of the jet exit, compares favorably to the actual flame front shown in Figure 1.

**Experimental composition and temperature measurements**

Composition and temperature measurements were taken in the reacting flow for the flow conditions represented by point B (Case 3) in order to compare experimental results to those predicted by the numerical program. The axial plane in which the composition and temperature measurements were made is illustrated schematically in Figure 8. (The combustor was insulated to simulate the adiabatic boundary conditions at the wall adopted in the numerical analysis.) Measurements were taken 1$\frac{1}{4}$ inches downstream of the jet exit (1-inch upstream of the exit plane of the combustor).

A water-cooled probe, $\frac{5}{8}$ inch in diameter was used for the composition measurements. The composition samples, drawn from the probe, were analyzed using a time-of-flight mass spectrometer (Bendix Model 17-210). The temperature was measured with a Pt/Pt-13 percent-Rh thermocouple mounted on a $\frac{1}{4}$ inch diameter ceramic probe. The
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ANALYTICAL AND EXPERIMENT RESULTS COMPARED

The constants $A$ and $E$ in the chemical rate expression (Equation 10) were refined by making use of the experimental results at point $A$ and $B$ in Figure 3. Initially, the pre-exponential factor, $A$, was modified to predict blowout for the approach velocity represented by point $A$ (Case 1). This procedure yielded a value for $A$ of $36 \times 10^{10}$.

The next step was directed toward refining the value of $E$, the activation energy. $E$ was modified to produce temperature and composition profiles with reasonable agreement to the experimentally measured profiles. The reduction in the activation energy was accompanied by a reduction in the pre-exponential factor $A$, ensuring that the blowout condition at point $A$ remained satisfied. The refinement of $A$ and $E$ resulted in the values given by equation 14.

The numerically predicted and experimentally measured profiles of fuel mole fraction and temperature are compared in Figure 9. The agreement is satisfactory from the combustor wall to a radius of 0.6-inch. The lower temperature and higher fuel mole fraction predicted numerically near the combustor wall is attributed to the assumption of a constant and uniform specific heat. For temperatures below the adiabatic flame temperature, the value taken for the specific heat is higher than the actual specific heat of the mixture. The wide spacing of the grid near the Vycor wall is also a contributing factor. The boundary condition for the fuel mole fraction at the wall assumes that the gradient is normal to the wall and that the distribution of temperature is parabolic near the wall. This boundary condition in conjunction with the few grid points near the wall serves to exaggerate the curvature of the profile adjacent to the wall.

The effect of the jet cooling is indicated by the experimental measurements of temperature near the jet. The numerical calculations assumed an adiabatic jet wall. The experimental measurements show that this assumption is not accurate. The results of the numerical program and experiment indicate that the heat-sink effect of the jet occurs at a critical point in the temperature history of the mixture.

To assess the effect on the numerical solution of assuming an adiabatic jet wall, a calculation was made with an isothermal jet wall. The choice of temperature for the jet wall was based on the experimental profile of temperature. An extrapolation of the temperature profile to the jet wall gives a value of about 1000 °F.

The profiles of temperature and composition for an isothermal jet wall at 1000 °F are given in Figure 10.† The results show the strong influence of the jet cooling on the temperature and composition profiles.

† The distributions of temperature and fuel mole fraction upstream of the jet presented in Figure 7 are unaffected when the jet wall is made adiabatic. Only the distributions near the jet wall are affected by the modified jet boundary condition.
of heat transfer on the predicted flowfield near the jet when compared to the profiles of Figure 9 and the importance of accurately prescribing the boundary conditions. The predicted temperature drops near the jet wall, consistent with the experimental profile. The predicted fuel mole fraction near the jet wall shows that the degree of reaction is less than that indicated in Figure 9 for an adiabatic wall. This result is consistent with the experimental observation.

The difference between the predicted and experimentally measured temperature near the wall is attributed in part to the radiation heat loss from the thermocouple. The temperature loss due to radiation is on the order of a few hundred degrees at the measured temperature of 1800 °F (Samuelsen, 1970). The difference between the predicted and experimentally measured fuel mole fraction is attributed to the simplified models of turbulence and chemical kinetics.

The assumption of an isothermal jet wall also contributes to the difference between the experimental and numerical results. The temperature variation along the jet wall may be significant. It should be emphasized that the present study is exploratory in nature. Little correlation has been previously attempted between numerical predictions and experimental measurements in turbulent, reacting flows with recirculation. The agreement between the numerical program and experimental work reported here is remarkably good considering the simple models used and the adoption of a constant and uniform specific heat. The results of this work demonstrate the potential of numerical calculation to predict the point-by-point properties of a reacting, turbulent flow and suggest that more extensive correlation to experiment should be conducted to develop and refine the numerical models used.

CONCLUSIONS

1. The governing equations for a reacting turbulent flow with recirculation can be solved with results consistent with experimental measurements.

2. Before the full utility of the solution procedure can be realized, more refined models of kinetics and turbulence must be developed and more extensive correlation to controlled experiment must be conducted.

3. Analytical results indicate a zone of near-homogeneous mixture and uniform temperature located downstream of the stagnation region of the opposed-reacting-jet.

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