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ANALYTICAL AND EXPERIMENTAL STUDY OF TURBULENT  
METHANE-FIRED BACKMIXED COMBUSTION

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# ANALYTICAL AND EXPERIMENTAL STUDY OF TURBULENT METHANE-FIRED BACKMIXED COMBUSTION\*

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## Abstract

Numerical predictions of the backmixed flowfield of a methane-fired laboratory combustor are compared to experimental observations. The goal is to clarify the mechanisms responsible for pollutant formation in continuous backmixed combustion and to improve predictive methods. The numerical description adopts a simplified effective viscosity model and a two-step kinetic reaction scheme for the methane oxidation. A reaction mechanism to account for the production of nitric oxide is also considered. Laser Doppler velocimetry is used to experimentally measure velocity profiles in the flowfield. Conventional gas sampling techniques are used to measure species concentration profiles.

## I. Introduction

Continuous combustion processes represent a category of combustion characterized by an un-interrupted, chemically reacting flow. Continuous combustion processes feature a complex interaction of chemical kinetics, heat transfer, mass diffusion and fluid mechanics. An important characteristic of continuous combustion systems is a zone of recirculating flow or backmixing. The zone serves as a mechanism for flame stabilization by back-mixing hot combustion products upstream to ignite incoming fresh reactants. Gas turbine engines, utility boilers and package boilers comprise the largest class of practical continuous combustion power sources.

Continuous combustion engineering design practices have traditionally been based on considerations of thermodynamic efficiency and heat transfer rates. Present operating constraints, e.g., exhaust composition and fuel economy, have necessitated a more detailed study of the processes occurring in the combustion system. Because the time-temperature history of the combustion process plays an important role in determining pollutant production and fuel combustion efficiency, prior knowledge of concentration, temperature and velocity distributions is especially valuable. As a result, the design and operation of continuous combustion systems can be facilitated by predictions of performance by way of an analytical model.

Theoretical analyses of combustion-chamber flows generally incorporate mathematical models of the combustion processes in a suitable numerical framework for solving the governing conservation equations. Detailed modeling of flows dominated

by backmixing necessitates solving the appropriate elliptic partial differential equations.

Progress in modeling continuous combustion systems has been hampered by the scarcity of detailed flowfield data for reacting, recirculating flows. Experimental data guide the development of numerical models of continuous combustion and provide a basis for their evaluation. A review of the state-of-the-art in continuous combustor modeling may be found in Osgerby (1974).<sup>1</sup>

This paper presents results from a continuing investigation designed to broaden the understanding of the physical and chemical processes occurring in turbulent combustion representative of practical systems. The governing equations describing a reacting, turbulent flowfield in a backmixed methane/air combustor are solved numerically. Experimental data are obtained and compared to the numerical description of the flowfield.

## II. Background

The experimental configuration adopted for the present study is a simplified laboratory burner consisting of a 2 in. diameter axisymmetric duct containing an aerodynamic (opposed-jet) flameholder as shown in Fig. 1. The opposed-jet combustor (OJC) provides a versatile bench-scale combustor exhibiting flame characteristics representative of practical combustion systems. The OJC utilizes a high velocity jet stream to back-mix the primary flow of reactants.\*\* The flame is stabilized near the stagnation region of the main and jet streams. The versatility of the opposed-jet combustor stems from the controlling influence of the jet composition and temperature on the reaction.

The numerical procedure used to solve the governing equations of the opposed-jet flowfield is based upon extended versions of the PISTEP method of Gosman et al (1969)<sup>2</sup>. The numerical procedure solves simultaneously the basic equations describing 2-D, elliptic flow with the corresponding dependent variables listed below:

conservations of mass.....streamfunction,  $\psi$   
conservation of momentum.....vorticity,  $\omega/r$   
conservation of energy.....enthalpy,  $h$   
species continuity.....mass fraction,  $m_j$

The OJC geometry has previously been incorporated into the computational procedure by Samuelsen and Starkman (1972).<sup>3</sup>

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\*\*The mass flow rate of the jet is much less than the mass flow rate of the main stream ( $\dot{m}_j/\dot{m}_p \ll 1$ ).



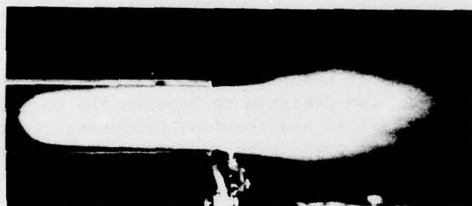
Turbulent transport properties (exchange coefficients) are evaluated using the time-mean or "effective" quantities. A simplified effective viscosity model was adopted for the present investigation<sup>2</sup>

$$\mu_{eff} = K D^{2/3} L^{-1/3} \rho^{2/3} (\dot{m} v^2)^{1/3} \quad (1)$$

Additional exchange coefficients are related to  $\mu_{eff}$  via the appropriate Prandtl or Schmidt number as follows:

$$\sigma_{h,eff} = \frac{\mu_{eff}}{\Gamma_{h,eff}} \quad \sigma_{m_j,eff} = \frac{\mu_{eff}}{\Gamma_{m_j,eff}} \quad (2)$$

a)



b)

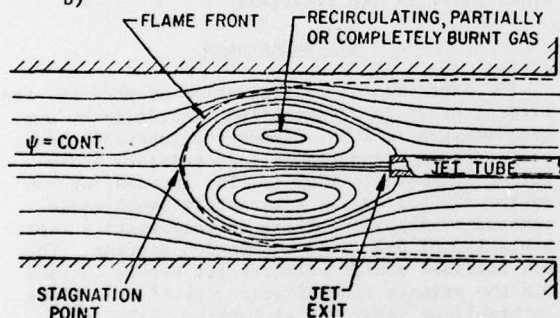


Figure 1 Opposed-jet Combustor  
a) photograph  
b) schematic of stream function distribution

### III. Approach

#### Cold Flow

Consideration of cold flow conditions enables a preliminary evaluation of the transport models incorporated into the numerical procedure. A cold flow solution is obtained by numerically solving the governing equations for the two dependent variables  $\psi, \omega$ . The predicted spatial distributions of the time-average (mean) velocity are available for comparison to the experimental measurements.

Distributions for the mean velocity are measured experimentally by using a laser Doppler velocimeter (LDV). The optical diagnostic technique is desirable because it does not disturb the characteristic

recirculating flowfield. The LDV is operated in a forward scatter real-fringe mode using a 5mW He-Ne laser light source and a DISA (Model 55L20) frequency tracker for Doppler signal processing. Additional features of the LDV system have been described previously.<sup>4</sup> Cold flow velocity data are used as a reference base for evaluating the system aerodynamics, the numerical predictive method, and the associated models of turbulence.

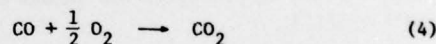
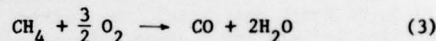
The effective mass exchange model may be evaluated by considering a cold flowfield with a non-uniform concentration. The nonuniform concentration is established by introduction of a tracer into the jet. Spatial distributions of tracer concentrations are predicted numerically by solving an additional species conservation equation containing the appropriate mass exchange coefficient.

Experimentally, a carbon monoxide (CO) tracer is introduced through the opposed-jet. Local CO concentrations are measured by NDIR analysis of gas samples extracted by conventional probing. Comparison of the predicted and experimentally determined distributions facilitate identification of deficiencies in the coupled mass exchange and effective viscosity models.

#### Reacting Flow

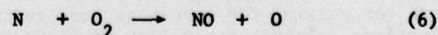
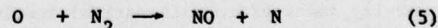
Calculated distributions of temperature and species mass fraction are compared to experimental results to assess the coupled models of turbulence and kinetics for the condition of reacting flow. The chemistry model incorporates kinetic mechanisms for methane, carbon monoxide and nitric oxide.

A two-step quasi-global reaction mechanism for methane oxidation<sup>5</sup> is adopted for the initial phase of the study:



A detailed description of the numerical formulation of the reaction rate expressions may be found in Samuelsen and Peck (1972).<sup>6</sup> The dependent variables for the hydrocarbon system include vorticity,  $\omega/r$ , streamfunction,  $\psi$ , methane mass fraction,  $m_{CH_4}$ , carbon dioxide mass fraction,  $m_{CO_2}$ , and enthalpy,  $\tilde{h}$ . Distributions of other major species  $H_2O$ , CO and  $O_2$  are related to  $m_{CH_4}$  and  $m_{CO_2}$  via elemental mass conservation.

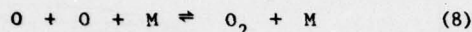
Additional calculations were conducted to predict formation of the pollutant species, nitric oxide (NO). Nitrogen oxide kinetics were based on the familiar Zeldovich<sup>7</sup> mechanism:



Noting that reaction (5) is the rate limiting step simplifies the overall reaction rate to:

$$\frac{d[\text{NO}]}{dt} = 2k_5 [\text{N}_2] [\text{O}] \quad (7)$$

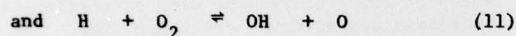
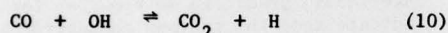
The problem remains to prescribe the O-atom concentration in Eq. (7). Two cases are considered in the present analysis. Equilibration of the elementary reaction



specifies the local O-atom concentration via the following expression:

$$\text{Case 1} \quad [\text{O}] = K_8 [\text{O}_2]^{1/2} \quad (9)$$

Recent evidence indicates that the assumption of  $\text{O}/\text{O}_2$  equilibrium underestimates the concentration of monatomic oxygen atoms.<sup>8-10</sup> The so-called "super-equilibrium" of oxygen atoms was incorporated into the NO kinetic expression following the method of Iverach et al. (1973).<sup>9</sup> By assuming that the reactions



are in equilibrium, the following expression for the concentration of oxygen atoms may be obtained:

$$\text{Case 2} \quad [\text{O}] = \frac{K_{10} K_{11} [\text{CO}][\text{O}_2]}{[\text{CO}_2]} \quad (12)$$

The experimental tests conducted to complement the numerical predictions of OJC reacting flow properties utilized stoichiometric proportions of premixed methane/air as reactants. Temperature and chemical composition measurements were obtained at the OJC exit plane. Temperature measurements were made using a Pt/Pt-13% Rh thermocouple. Gas samples were extracted via a water-cooled stainless steel probe and conveyed through a heated teflon sample line to a packaged exhaust gas analysis system. The instrumentation console provides quantitative analyses of CO and  $\text{CO}_2$  (NDIR), NO/NO<sub>x</sub> (chemiluminescence), total hydrocarbons (FID), and  $\text{O}_2$  (paramagnetic).

#### IV. Results and Discussion

##### Cold Flow

The cold flow studies were conducted for the following test conditions:

Approach velocity  $V_m = 25$  fps

Jet velocity  $V_j = 425$  fps

Temperature  $T_m = T_j = 530^\circ\text{R}$

Equivalence Ratio,  $\frac{F/A_{\text{act}}}{F/A_{\text{stoich}}} \quad \phi_m = \phi_j = 0.0$

Experimental and predicted velocity profiles are presented in Fig. 2. The selected profiles emphasize the flow regime dominated by recirculation.

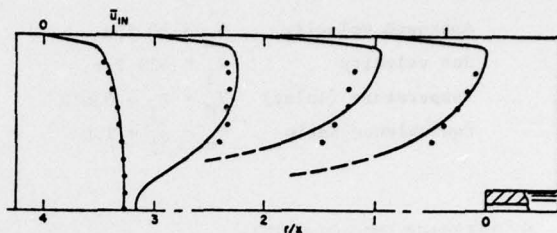
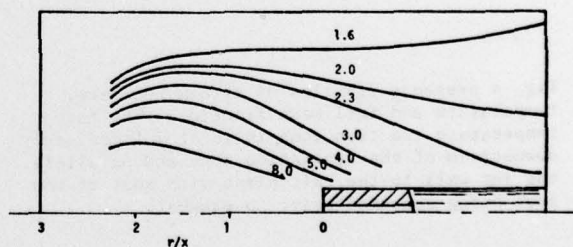


Fig. 2 Cold Flow Velocity Profiles  
(• exptl., -pred)

The predicted velocity profiles agree qualitatively with experimental results. The predicted location of the stagnation point differs substantially from the location indicated experimentally. The intense mixing processes occurring in the recirculation zone suggest employing a refined model of turbulence (eg. two parameter) based on the turbulent kinetic energy and a prescribed mixing length. A thorough evaluation is currently limited by the inability to experimentally obtain LDV measurements in the highly turbulent shear layer between the jet and the main stream or in the recirculation zone itself.

Results of the tracer studies of mass transport in a turbulent, nonreacting flow are shown in Fig. 3. Although the reported trends are similar, the calculated tracer concentration profiles are quantitatively higher than those observed experimentally. These results demonstrate deficiencies in the mass exchange coefficient and more importantly in the simplified effective viscosity model used in the current study.

##### a) %CO Predicted



##### b) %CO Experimental

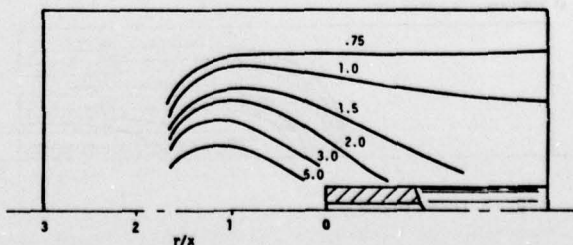


Fig. 3 Cold Flow Tracer Concentration Profiles



### Reacting Flow

Results of the reacting flow solution for the OJC are presented in Figs. 4 and 5. The conditions investigated for the hot flow case were as follows:

Approach velocity	$V_m = 50$ fps
Jet velocity	$V_j = 425$ fps
Temperature (inlet)	$T_m = T_j = 530^\circ\text{R}$
Equivalence Ratio	$\phi_m = \phi_j = 1.0$

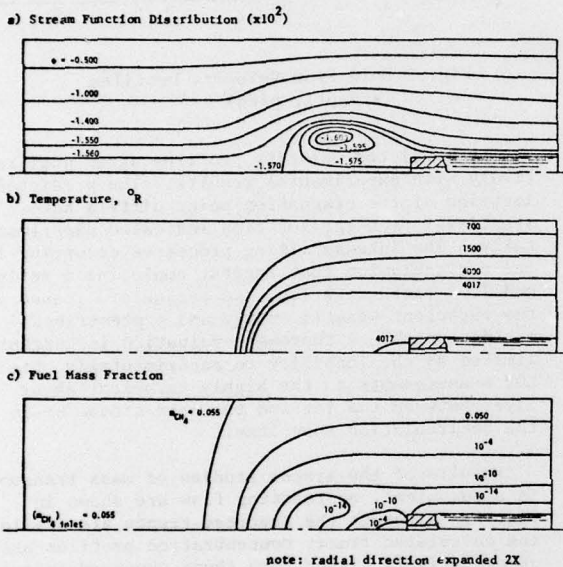


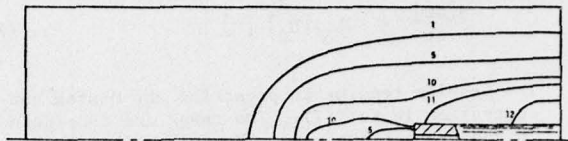
Fig. 4 Hot Flowfield Property Distributions (Predicted)

Fig. 4 presents profiles of stream function, temperature and fuel mass fraction. The high temperature reaction zone is located immediately downstream of the stagnation zone and parallels the jet wall to the exit plane with most of the fuel being consumed prior to exhaust.



Fig. 5 (continued)

b) PPM Nitric Oxide (NO): Case 1 O/O<sub>2</sub> Eqbrm.



c) PPM Nitric Oxide (NO): Case 2 O/O<sub>2</sub> Non-eqbrm.



note: radial direction expanded 2X

Fig. 5 Hot Flowfield Property Distributions (Predicted)

Predicted concentration profiles of the pollutant species CO and NO are shown in Fig. 5. Significant CO concentrations persist throughout the flame zone and reach a maximum in the transition (flame front) region where the temperature and oxygen concentration are relatively low. The numerically predicted NO profiles for Case 1 indicate that the maximum concentrations appear in the peak temperature zone with proportionate increases depending on residence time. The non-equilibrium condition of Case 2 results in a 30-fold increase in NO production.

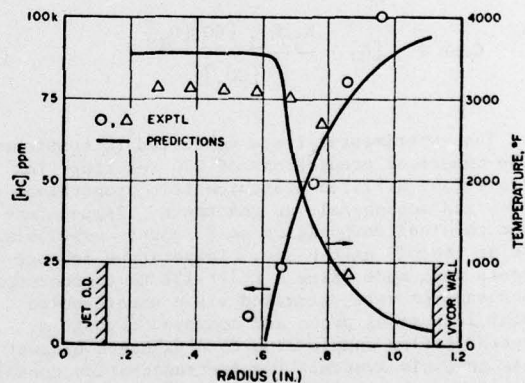


Fig. 6 OJC Exhaust HC and Temperature Profiles

Exhaust plane measurements of temperature and hydrocarbon concentration are compared to predicted values in Fig. 6. The location of the flame front, indicated by steep temperature and concentration gradients, coincides with theoretical predictions. The temperature deviation in the reaction zone may be corrected by considering radiation losses in both the numerical and experimental results.

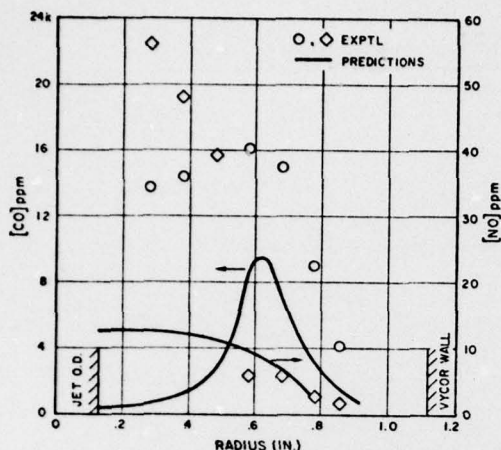


Fig. 7 OJC Exhaust CO and NO Profiles

Fig. 7 presents similar results for CO and Case 1 NO concentrations. The indicated trends are favorable, but the magnitude of predicted CO and NO levels are significantly low. Examining the controlling kinetic rate models indicates that the conversion of  $\text{CO} \rightarrow \text{CO}_2$  does not occur as rapidly as Eq. (4) predicts.<sup>2</sup> The observed NO levels exceed those predicted via the Zeldovich mechanism with  $\text{O}/\text{O}_2$  equilibrium, yet fall well below the non-equilibrium calculations.

In general, the analytical treatment of OJC reacting flows produced results simulating gross flame characteristics. The coupled turbulent/kinetic models adopted for the initial calculations require further refinements before adequate experimental correlation is achieved.

#### V. Summary

Numerical predictions of the turbulent, back-mixed flowfield of a methane-fired opposed-jet combustor have been compared to experimental observations. Although, favorable qualitative correlation has been established, deficiencies in the predictive models have been identified. A cold flow analysis identified deficiencies in the simplified turbulence model considered. A hot flow analysis identified deficiencies in the coupled turbulent/kinetic models adopted. The results from this preliminary study provide a reference base for further experimental verification and formulation of refined kinetic and transport mechanisms.

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#### VII. Nomenclature

D	combustor diameter
$\tilde{h}$	stagnation enthalpy
K	constant in effective viscosity expression
$K_i$	equilibrium constant
$k_i$	kinetic rate constant
L	length of flowfield
$\dot{m}$	mass flow rate
$m_j$	mass fraction of jth species
r	radius
T	temperature
v	velocity
$\Gamma$	exchange coefficient
$\mu$	viscosity
$\rho$	density
$\sigma_j$	Schmidt Number
$\sigma_h$	Prandtl Number
$\phi$	equivalence ratio
$\psi$	stream function
$\omega$	vorticity
[i]	concentration of species i



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